Full wwPDB X-ray Structure Validation Report (i)

May 23, 2016 – 07:58 PM EDT

PDB ID	:	1KIJ
Title	:	Crystal structure of the 43K ATPase domain of Thermus thermophilus gyrase B in complex with novobiocin
Authors	:	Lamour, V.; Hoermann, L.; Jeltsch, J.-M.; Oudet, P.; Moras, D.
Deposited on	:	2001-12-03
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:

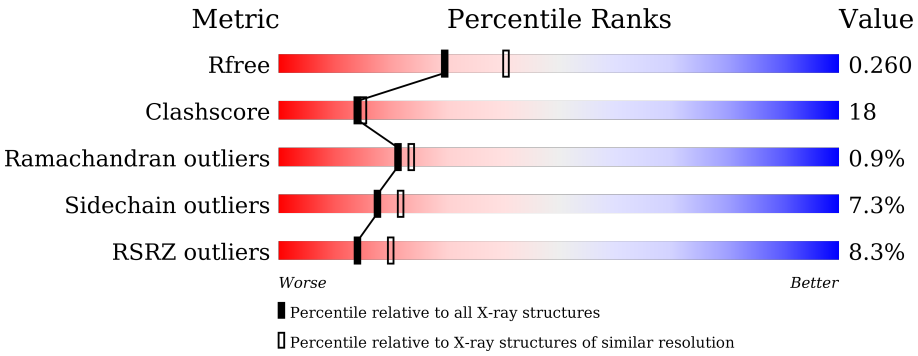
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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	390	9% 69% 25%
1	B	390	8% 69% 25%

2 Entry composition

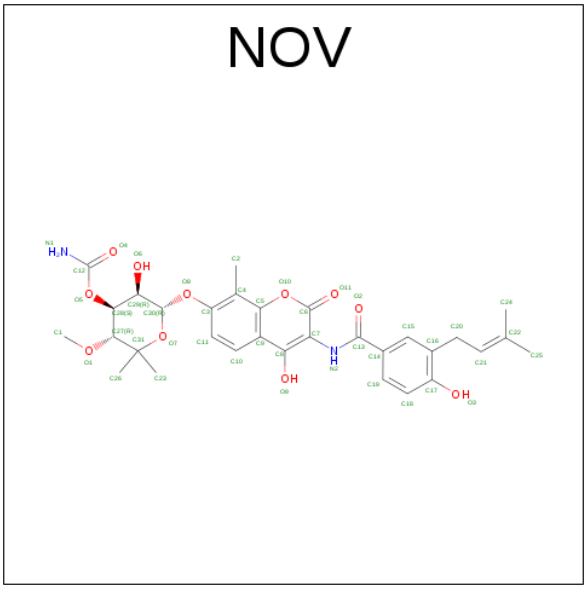
There are 4 unique types of molecules in this entry. The entry contains 6498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA GYRASE SUBUNIT B.

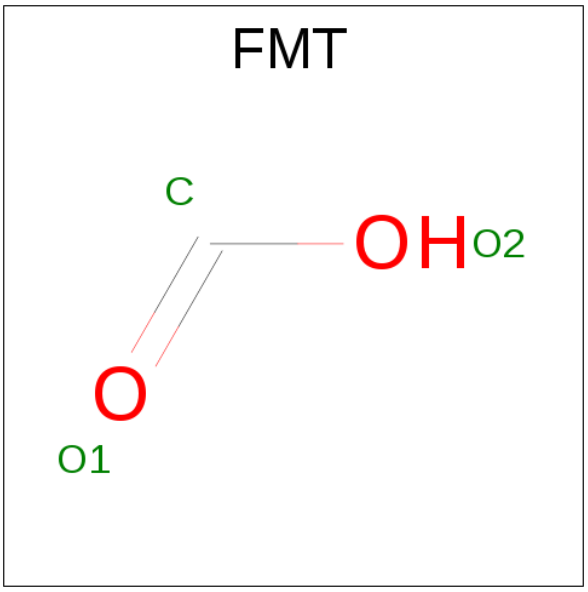
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2968	1881	530	554	3			
1	B	384	Total	C	N	O	S	0	0	0
			2968	1881	530	554	3			

- Molecule 2 is NOVOBIOCIN (three-letter code: NOV) (formula: $C_{31}H_{36}N_2O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	31	2	11		
2	B	1	Total	C	N	O	0	0
			44	31	2	11		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 4 is water.

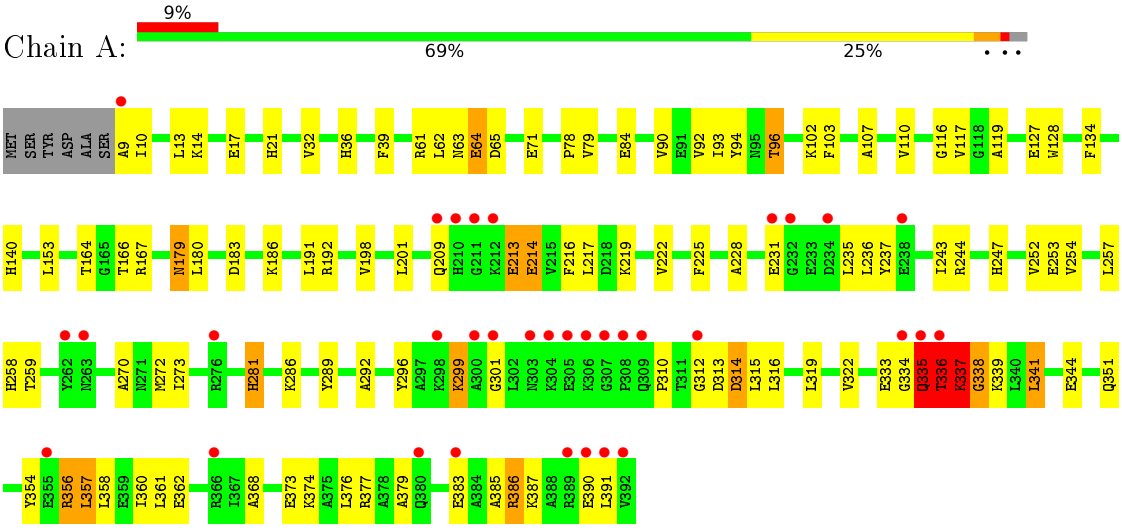
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	228	Total O 228 228	0	0
4	B	240	Total O 240 240	0	0

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.

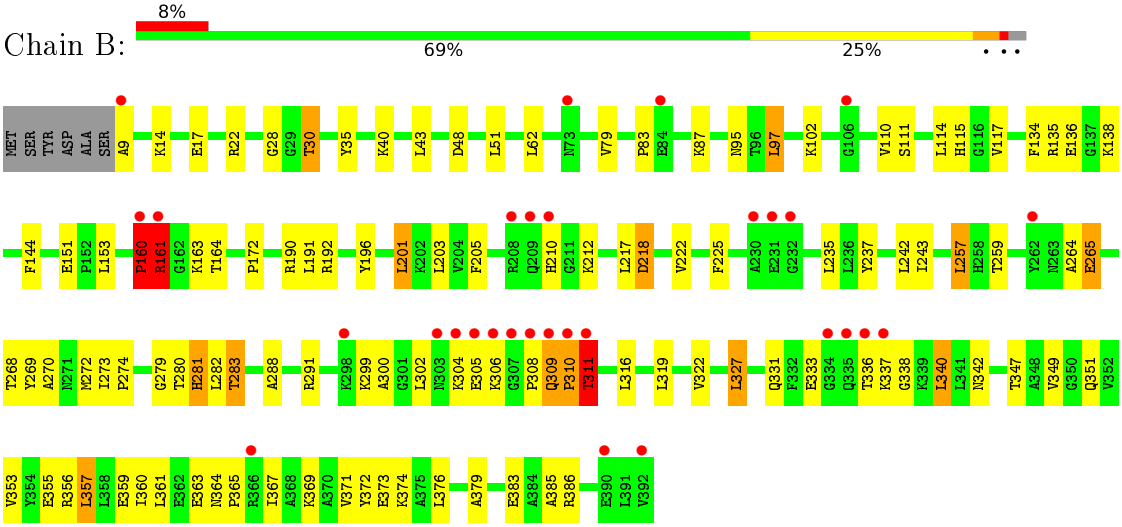
- Molecule 1: DNA GYRASE SUBUNIT B

Chain A:



- Molecule 1: DNA GYRASE SUBUNIT B

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.88Å 125.55Å 79.83Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	14.94 – 2.30 14.94 – 2.31	Depositor EDS
% Data completeness (in resolution range)	94.9 (14.94-2.30) 95.0 (14.94-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.35 (at 2.32Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.266 0.204 , 0.260	Depositor DCC
R_{free} test set	2765 reflections (7.54%)	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6498	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FMT, NOV

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	0.48	1/3025 (0.0%)	0.66	4/4086 (0.1%)
1	B	0.52	2/3025 (0.1%)	0.65	4/4086 (0.1%)
All	All	0.50	3/6050 (0.0%)	0.65	8/8172 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	ARG	N-CA	18.61	1.83	1.46
1	A	338	GLY	N-CA	16.30	1.70	1.46
1	B	311	THR	N-CA	6.85	1.60	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	GLY	N-CA-C	-10.53	86.77	113.10
1	A	335	GLN	C-N-CA	8.47	142.86	121.70
1	B	161	ARG	N-CA-CB	8.27	125.48	110.60
1	B	160	PRO	C-N-CA	-8.02	101.66	121.70
1	B	311	THR	N-CA-C	-7.71	90.19	111.00
1	A	337	LYS	C-N-CA	-7.00	107.59	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	ASP	N-CA-C	-6.12	94.48	111.00
1	B	311	THR	N-CA-CB	5.46	120.67	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	GLN	Peptide
1	A	337	LYS	Peptide
1	B	160	PRO	Peptide

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	2968	0	2985	113	0
1	B	2968	0	2985	115	0
2	A	44	0	35	5	0
2	B	44	0	36	1	0
3	A	3	0	2	0	0
3	B	3	0	2	0	0
4	A	228	0	0	7	0
4	B	240	0	0	10	0
All	All	6498	0	6045	221	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 18.

All (221) 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:338:GLY:CA	1:A:338:GLY:N	1.70	1.52
1:B:161:ARG:CA	1:B:161:ARG:N	1.83	1.41
1:B:331:GLN:H	1:B:342:ASN:HD21	1.09	0.98
1:A:334:GLY:O	1:A:335:GLN:HG2	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:VAL:O	1:B:353:VAL:HG12	1.66	0.93
1:A:243:ILE:HB	1:A:254:VAL:HG13	1.50	0.93
1:A:338:GLY:N	1:A:338:GLY:C	2.21	0.93
1:A:335:GLN:NE2	1:A:337:LYS:O	2.03	0.92
1:A:36:HIS:HE1	1:A:183:ASP:H	1.19	0.88
1:B:161:ARG:N	1:B:161:ARG:HA	1.87	0.87
1:A:337:LYS:C	1:A:338:GLY:CA	2.45	0.85
1:B:161:ARG:NH1	1:B:163:LYS:HD2	1.92	0.84
1:B:279:GLY:O	1:B:283:THR:HG22	1.78	0.83
1:B:160:PRO:C	1:B:161:ARG:CA	2.47	0.82
1:B:201:LEU:HD13	1:B:203:LEU:HD11	1.60	0.82
1:A:235:LEU:HD13	1:A:257:LEU:HD21	1.62	0.81
1:B:161:ARG:HH12	1:B:163:LYS:HD2	1.44	0.80
1:A:333:GLU:HG2	1:A:341:LEU:HD21	1.61	0.80
1:B:161:ARG:CZ	1:B:163:LYS:HB2	2.11	0.80
1:B:280:THR:HG21	1:B:342:ASN:O	1.83	0.78
1:B:235:LEU:HD22	1:B:257:LEU:HD21	1.66	0.78
1:A:36:HIS:CE1	1:A:183:ASP:H	2.05	0.74
1:A:236:LEU:O	1:A:236:LEU:HD23	1.91	0.71
1:B:161:ARG:NH2	1:B:163:LYS:HD2	2.06	0.71
1:A:243:ILE:HB	1:A:254:VAL:CG1	2.21	0.70
1:B:222:VAL:HG13	1:B:322:VAL:HB	1.74	0.70
1:B:161:ARG:CZ	1:B:163:LYS:HD2	2.21	0.70
1:B:160:PRO:O	4:B:831:HOH:O	2.10	0.70
1:A:92:VAL:O	1:A:96:THR:HG23	1.92	0.69
1:A:338:GLY:N	1:A:339:LYS:N	2.40	0.69
1:A:334:GLY:HA2	1:B:28:GLY:HA3	1.73	0.69
1:A:9:ALA:HB1	4:B:913:HOH:O	1.92	0.69
1:A:65:ASP:HB3	4:A:916:HOH:O	1.91	0.69
1:A:313:ASP:HA	1:A:316:LEU:HG	1.74	0.68
1:B:336:THR:O	1:B:337:LYS:HG3	1.94	0.68
1:A:333:GLU:O	1:A:335:GLN:OE1	2.12	0.68
1:B:243:ILE:HD11	1:B:360:ILE:HD12	1.75	0.68
1:B:161:ARG:HG3	1:B:163:LYS:N	2.08	0.67
1:B:309:GLN:HG2	1:B:310:PRO:HD3	1.77	0.67
1:B:161:ARG:HG3	1:B:163:LYS:H	1.60	0.67
1:A:334:GLY:C	1:A:335:GLN:HG2	2.15	0.65
1:A:107:ALA:HB1	4:A:595:HOH:O	1.95	0.65
1:B:161:ARG:HH22	1:B:163:LYS:HD2	1.62	0.64
1:A:228:ALA:HA	1:A:231:GLU:HG3	1.79	0.64
1:B:309:GLN:CG	1:B:310:PRO:HD3	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HD22	1:A:179:ASN:C	2.01	0.63
1:B:243:ILE:HD12	1:B:356:ARG:HG3	1.79	0.62
1:B:369:LYS:O	1:B:373:GLU:HB2	2.00	0.62
1:A:222:VAL:CG2	1:A:322:VAL:HB	2.30	0.61
1:B:367:ILE:O	1:B:371:VAL:HG12	2.00	0.61
1:B:30:THR:CG2	1:B:30:THR:O	2.49	0.60
1:B:309:GLN:HG2	1:B:310:PRO:CD	2.31	0.60
1:B:160:PRO:O	1:B:161:ARG:O	2.19	0.60
1:B:308:PRO:HA	4:B:837:HOH:O	2.01	0.60
1:B:243:ILE:HD12	1:B:356:ARG:CG	2.31	0.60
1:A:102:LYS:HD2	1:B:9:ALA:CB	2.32	0.59
1:A:335:GLN:CD	1:A:337:LYS:O	2.41	0.59
1:A:391:LEU:HD23	1:A:391:LEU:O	2.01	0.59
1:A:244:ARG:HG2	1:A:253:GLU:HG2	1.84	0.59
1:B:333:GLU:OE2	1:B:338:GLY:HA3	2.01	0.59
1:B:331:GLN:H	1:B:342:ASN:ND2	1.90	0.58
1:B:379:ALA:O	1:B:383:GLU:HG3	2.03	0.58
1:B:135:ARG:HG2	1:B:136:GLU:HG3	1.85	0.57
1:A:273:ILE:HD12	1:A:273:ILE:O	2.04	0.57
1:A:247:HIS:CD2	1:A:351:GLN:HG2	2.38	0.57
1:A:79:VAL:HG12	1:A:90:VAL:HG21	1.86	0.57
1:B:268:THR:HG21	1:B:282:LEU:HB2	1.85	0.57
1:A:386:ARG:HD3	1:A:386:ARG:C	2.26	0.56
1:A:296:TYR:CE2	1:A:368:ALA:HB1	2.40	0.56
1:B:386:ARG:HH11	1:B:386:ARG:HB3	1.70	0.56
1:A:259:THR:O	1:A:374:LYS:HE2	2.04	0.56
1:A:102:LYS:HD2	1:B:9:ALA:HB1	1.87	0.56
1:B:288:ALA:CB	1:B:353:VAL:HG13	2.36	0.55
1:A:335:GLN:CG	1:A:337:LYS:O	2.55	0.55
1:B:95:ASN:HD21	1:B:144:PHE:HE2	1.55	0.55
1:A:387:LYS:HA	1:A:390:GLU:OE2	2.06	0.55
1:A:93:ILE:HG23	1:A:117:VAL:HG11	1.90	0.53
1:B:304:LYS:O	1:B:305:GLU:HB3	2.08	0.53
1:A:134:PHE:O	1:A:164:THR:HA	2.07	0.53
1:A:299:LYS:HE2	1:A:299:LYS:HA	1.90	0.53
1:B:97:LEU:HD22	1:B:115:HIS:CD2	2.43	0.53
1:B:340:LEU:HD22	1:B:342:ASN:HD22	1.73	0.53
1:A:247:HIS:HD2	1:A:351:GLN:HG2	1.74	0.53
1:B:161:ARG:NH1	1:B:163:LYS:CD	2.67	0.53
1:B:331:GLN:N	1:B:342:ASN:HD21	1.93	0.53
1:A:32:VAL:O	1:A:36:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLN:CD	1:B:310:PRO:HD3	2.30	0.52
1:B:300:ALA:HB3	1:B:302:LEU:HD13	1.91	0.52
1:A:110:VAL:HG22	1:A:272:MET:HG3	1.91	0.51
1:A:140:HIS:HB3	1:A:153:LEU:HD11	1.93	0.51
1:B:14:LYS:O	1:B:17:GLU:HB2	2.10	0.51
1:B:310:PRO:O	1:B:311:THR:HG23	2.08	0.51
1:A:217:LEU:HD23	1:A:217:LEU:C	2.30	0.51
1:B:363:GLU:C	1:B:365:PRO:HD3	2.31	0.51
1:A:335:GLN:HG3	1:A:337:LYS:O	2.10	0.51
1:A:386:ARG:HD3	1:A:386:ARG:O	2.11	0.50
1:A:373:GLU:O	1:A:377:ARG:HG3	2.12	0.50
1:A:312:GLY:O	1:A:313:ASP:HB2	2.10	0.50
1:A:383:GLU:HA	1:A:383:GLU:OE2	2.12	0.50
1:B:310:PRO:O	1:B:311:THR:OG1	2.26	0.50
1:A:127:GLU:HG3	1:A:128:TRP:CD1	2.45	0.50
1:A:228:ALA:O	1:A:231:GLU:HG3	2.11	0.50
1:B:281:HIS:H	1:B:281:HIS:CD2	2.30	0.50
1:B:79:VAL:HB	1:B:153:LEU:HD21	1.92	0.50
1:A:358:LEU:O	1:A:362:GLU:HG3	2.12	0.50
1:A:387:LYS:O	1:A:390:GLU:HG2	2.11	0.50
1:B:243:ILE:HD11	1:B:360:ILE:CD1	2.41	0.50
1:A:354:TYR:O	1:A:358:LEU:HD23	2.11	0.50
1:B:270:ALA:O	1:B:273:ILE:HG12	2.11	0.50
1:B:309:GLN:HB3	1:B:376:LEU:HD21	1.93	0.49
1:A:102:LYS:CD	1:B:9:ALA:HB1	2.42	0.49
1:A:289:TYR:CD1	1:A:357:LEU:HD11	2.48	0.49
1:B:210:HIS:HB3	1:B:212:LYS:HE3	1.94	0.49
1:A:281:HIS:CD2	1:A:281:HIS:H	2.32	0.48
1:B:161:ARG:NH2	1:B:163:LYS:HG3	2.29	0.48
1:A:79:VAL:HG12	1:A:90:VAL:CG2	2.42	0.48
1:B:161:ARG:NH2	1:B:163:LYS:CG	2.77	0.47
1:B:309:GLN:HG3	1:B:372:TYR:CE1	2.49	0.47
1:A:93:ILE:HD11	2:A:400:NOV:C24	2.44	0.47
1:A:78:PRO:O	1:A:90:VAL:HG22	2.14	0.47
1:B:161:ARG:NH2	1:B:163:LYS:CD	2.75	0.47
1:B:83:PRO:HG2	4:B:880:HOH:O	2.13	0.47
1:A:314:ASP:OD2	1:A:379:ALA:HA	2.15	0.47
1:B:43:LEU:C	1:B:43:LEU:HD13	2.35	0.47
1:B:161:ARG:CZ	1:B:163:LYS:CB	2.88	0.47
1:A:93:ILE:HD13	2:A:400:NOV:H233	1.97	0.47
1:B:269:TYR:HE2	1:B:274:PRO:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PRO:O	1:B:161:ARG:C	2.53	0.46
1:B:196:TYR:HE2	1:B:218:ASP:OD1	1.99	0.46
1:A:179:ASN:ND2	1:A:179:ASN:C	2.68	0.46
1:B:347:THR:O	1:B:351:GLN:HB2	2.16	0.46
1:B:40:LYS:HD3	4:B:934:HOH:O	2.16	0.46
1:A:313:ASP:HA	1:A:316:LEU:CG	2.44	0.46
1:B:35:TYR:CE1	1:B:172:PRO:HB2	2.51	0.45
1:A:61:ARG:HD2	1:A:63:ASN:OD1	2.15	0.45
1:A:10:ILE:HD11	2:B:444:NOV:C22	2.46	0.45
1:A:222:VAL:HG22	1:A:322:VAL:HB	1.97	0.45
1:A:361:LEU:HD12	1:A:368:ALA:CB	2.47	0.45
1:B:217:LEU:HD23	1:B:218:ASP:N	2.32	0.45
1:B:222:VAL:HG13	1:B:322:VAL:CB	2.45	0.45
1:A:64:GLU:HG2	1:A:64:GLU:H	1.53	0.45
1:A:65:ASP:HB3	4:A:931:HOH:O	2.16	0.45
1:B:160:PRO:O	1:B:161:ARG:CA	2.63	0.45
1:A:198:VAL:HG23	1:A:272:MET:HE1	1.98	0.45
1:A:270:ALA:O	1:A:273:ILE:HG13	2.17	0.45
1:A:310:PRO:HG3	1:A:376:LEU:HD23	1.98	0.45
1:A:94:TYR:CE2	1:A:119:ALA:HB1	2.52	0.45
1:A:336:THR:HG22	4:A:841:HOH:O	2.16	0.45
1:A:357:LEU:HD22	1:A:361:LEU:CD2	2.46	0.45
1:A:214:GLU:HG2	1:A:216:PHE:CZ	2.52	0.45
1:A:258:HIS:CE1	1:A:319:LEU:HD13	2.51	0.45
1:B:190:ARG:HD3	4:B:918:HOH:O	2.17	0.45
1:A:357:LEU:HD22	1:A:361:LEU:HD21	1.98	0.45
1:A:273:ILE:C	1:A:273:ILE:HD12	2.36	0.45
1:A:93:ILE:HD11	2:A:400:NOV:H241	1.98	0.45
1:B:48:ASP:OD1	1:B:110:VAL:HG23	2.17	0.44
1:B:192:ARG:HD3	4:B:562:HOH:O	2.17	0.44
1:B:134:PHE:O	1:B:164:THR:HA	2.18	0.44
1:B:201:LEU:HD13	1:B:203:LEU:CD1	2.41	0.44
1:B:51:LEU:HD11	1:B:272:MET:HE3	1.99	0.44
1:B:310:PRO:HD2	4:B:837:HOH:O	2.17	0.44
1:B:288:ALA:HB1	1:B:353:VAL:HG13	2.00	0.44
1:A:192:ARG:HD3	4:A:887:HOH:O	2.17	0.44
1:A:214:GLU:HG2	1:A:216:PHE:CE2	2.53	0.44
1:A:316:LEU:O	1:A:316:LEU:HD12	2.18	0.44
1:A:32:VAL:CG1	1:A:186:LYS:HE3	2.48	0.44
1:B:161:ARG:NH1	1:B:163:LYS:HB2	2.32	0.44
1:B:87:LYS:HG2	4:B:897:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:PRO:O	1:B:311:THR:CB	2.65	0.44
1:B:30:THR:O	1:B:30:THR:HG22	2.18	0.43
1:B:264:ALA:O	1:B:265:GLU:HB2	2.18	0.43
1:B:264:ALA:HB2	1:B:316:LEU:O	2.18	0.43
1:B:161:ARG:CZ	1:B:163:LYS:CD	2.95	0.43
1:A:14:LYS:O	1:A:17:GLU:HG3	2.18	0.43
1:A:333:GLU:HB2	1:A:335:GLN:OE1	2.18	0.43
1:B:237:TYR:CD1	1:B:237:TYR:O	2.72	0.43
1:B:265:GLU:OE2	1:B:265:GLU:HA	2.18	0.43
1:B:364:ASN:N	1:B:365:PRO:HD3	2.34	0.43
1:B:243:ILE:CD1	1:B:356:ARG:HG3	2.48	0.43
1:A:13:LEU:HD11	1:A:21:HIS:CD2	2.53	0.43
1:B:309:GLN:HG3	1:B:372:TYR:HE1	1.84	0.43
1:A:79:VAL:HB	1:A:153:LEU:HD21	2.01	0.43
1:B:117:VAL:HG22	4:B:808:HOH:O	2.17	0.43
1:A:102:LYS:HD2	1:B:9:ALA:HB2	1.99	0.42
1:A:356:ARG:O	1:A:360:ILE:HG12	2.19	0.42
1:B:309:GLN:HB3	1:B:376:LEU:CD2	2.50	0.42
1:A:110:VAL:HG13	1:A:272:MET:HB2	2.02	0.42
1:A:213:GLU:HB2	4:A:901:HOH:O	2.18	0.42
1:A:228:ALA:CA	1:A:231:GLU:HG3	2.49	0.42
1:A:237:TYR:O	1:A:257:LEU:HD11	2.19	0.42
1:B:359:GLU:O	1:B:363:GLU:HG2	2.20	0.42
1:B:327:LEU:N	1:B:327:LEU:HD12	2.35	0.42
1:A:333:GLU:HG2	1:A:341:LEU:CD2	2.41	0.42
1:B:257:LEU:C	1:B:257:LEU:HD23	2.41	0.42
1:A:237:TYR:HE1	1:A:258:HIS:HB2	1.85	0.42
1:B:138:LYS:HB2	1:B:138:LYS:HE3	1.83	0.42
1:B:259:THR:O	1:B:374:LYS:HE3	2.20	0.42
1:A:71:GLU:CD	1:A:167:ARG:HD3	2.39	0.41
1:A:313:ASP:CA	1:A:316:LEU:HG	2.46	0.41
1:B:305:GLU:C	1:B:306:LYS:HG2	2.40	0.41
1:A:237:TYR:CE2	1:A:257:LEU:HD12	2.55	0.41
1:A:286:LYS:HE2	1:A:286:LYS:HB3	1.82	0.41
1:A:387:LYS:HE2	4:A:871:HOH:O	2.20	0.41
1:B:191:LEU:HD23	1:B:205:PHE:HB2	2.02	0.41
1:B:111:SER:O	1:B:273:ILE:HG21	2.19	0.41
1:A:385:ALA:HB1	1:B:385:ALA:HB1	2.01	0.41
1:A:237:TYR:CE1	1:A:258:HIS:HB2	2.55	0.41
1:A:292:ALA:HB1	1:A:358:LEU:HD22	2.02	0.41
1:B:30:THR:O	1:B:30:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:H	1:A:344:GLU:CD	2.24	0.41
1:A:64:GLU:HA	1:A:209:GLN:HG3	2.02	0.41
1:B:191:LEU:CD2	1:B:205:PHE:HB2	2.51	0.41
1:B:222:VAL:CG1	1:B:322:VAL:HB	2.48	0.41
1:A:373:GLU:HA	1:A:376:LEU:HD12	2.03	0.41
1:B:269:TYR:CE2	1:B:274:PRO:HG3	2.56	0.41
1:B:340:LEU:CD2	1:B:342:ASN:HD22	2.32	0.41
1:B:353:VAL:O	1:B:357:LEU:HB2	2.20	0.41
1:A:166:THR:HB	2:A:400:NOV:HN11	1.86	0.40
1:A:116:GLY:HA2	1:B:22:ARG:NH2	2.36	0.40
1:A:333:GLU:CG	1:A:341:LEU:HD11	2.51	0.40
1:A:103:PHE:HB2	2:A:400:NOV:H10	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	382/390 (98%)	363 (95%)	17 (4%)	2 (0%)	34	41
1	B	382/390 (98%)	356 (93%)	21 (6%)	5 (1%)	15	15
All	All	764/780 (98%)	719 (94%)	38 (5%)	7 (1%)	21	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	THR
1	A	336	THR
1	B	160	PRO
1	B	161	ARG
1	B	265	GLU
1	A	301	GLY

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Mol	Chain	Res	Type
1	B	310	PRO

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	303/308 (98%)	281 (93%)	22 (7%)	17	22
1	B	303/308 (98%)	281 (93%)	22 (7%)	17	22
All	All	606/616 (98%)	562 (93%)	44 (7%)	17	22

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PHE
1	A	62	LEU
1	A	64	GLU
1	A	84	GLU
1	A	96	THR
1	A	179	ASN
1	A	180	LEU
1	A	191	LEU
1	A	201	LEU
1	A	213	GLU
1	A	214	GLU
1	A	219	LYS
1	A	225	PHE
1	A	252	VAL
1	A	281	HIS
1	A	299	LYS
1	A	315	LEU
1	A	336	THR
1	A	341	LEU
1	A	356	ARG
1	A	357	LEU
1	A	386	ARG

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Mol	Chain	Res	Type
1	B	30	THR
1	B	62	LEU
1	B	97	LEU
1	B	102	LYS
1	B	114	LEU
1	B	151	GLU
1	B	201	LEU
1	B	218	ASP
1	B	225	PHE
1	B	242	LEU
1	B	257	LEU
1	B	281	HIS
1	B	283	THR
1	B	291	ARG
1	B	299	LYS
1	B	309	GLN
1	B	319	LEU
1	B	327	LEU
1	B	340	LEU
1	B	355	GLU
1	B	357	LEU
1	B	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	36	HIS
1	A	45	ASN
1	A	95	ASN
1	A	179	ASN
1	A	210	HIS
1	A	247	HIS
1	A	281	HIS
1	A	295	GLN
1	A	335	GLN
1	A	351	GLN
1	A	380	GLN
1	B	45	ASN
1	B	73	ASN
1	B	209	GLN
1	B	210	HIS

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Mol	Chain	Res	Type
1	B	281	HIS
1	B	295	GLN
1	B	309	GLN
1	B	342	ASN

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

4 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	NOV	A	400	-	42,47,47	1.65	7 (16%)	53,70,70	2.29	18 (33%)
3	FMT	A	401	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	441	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NOV	B	444	-	42,47,47	1.19	2 (4%)	53,70,70	2.22	12 (22%)

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	NOV	A	400	-	-	0/23/46/46	0/4/4/4
3	FMT	A	401	-	-	0/0/0/0	0/0/0/0
3	FMT	B	441	-	-	0/0/0/0	0/0/0/0
2	NOV	B	444	-	-	0/23/46/46	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NOV	O7-C31	-4.25	1.41	1.46
2	B	444	NOV	O7-C31	-3.49	1.42	1.46
2	A	400	NOV	O6-C29	-2.41	1.37	1.43
2	A	400	NOV	C31-C27	2.60	1.57	1.52
2	A	400	NOV	C17-C16	2.61	1.43	1.40
2	B	444	NOV	O5-C28	2.72	1.48	1.44
2	A	400	NOV	C28-C27	2.97	1.58	1.52
2	A	400	NOV	C19-C14	3.05	1.44	1.39
2	A	400	NOV	O5-C28	5.39	1.52	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	NOV	O8-C30-C29	-5.31	99.37	106.98
2	B	444	NOV	O8-C30-C29	-4.77	100.13	106.98
2	B	444	NOV	O4-C12-N1	-4.50	117.22	125.50
2	A	400	NOV	C20-C21-C22	-4.14	122.71	127.72
2	A	400	NOV	C19-C18-C17	-3.57	116.92	120.50
2	B	444	NOV	C26-C31-C27	-3.27	106.12	112.01
2	A	400	NOV	O10-C5-C9	-2.99	118.06	121.21
2	A	400	NOV	O2-C13-N2	-2.57	117.93	123.68
2	A	400	NOV	O4-C12-N1	-2.50	120.90	125.50
2	A	400	NOV	C20-C16-C15	-2.50	115.19	120.75
2	A	400	NOV	C11-C10-C9	-2.47	117.89	121.15
2	B	444	NOV	O2-C13-N2	-2.33	118.47	123.68
2	B	444	NOV	C29-C28-C27	-2.15	106.94	110.43
2	B	444	NOV	O10-C5-C9	-2.14	118.95	121.21
2	B	444	NOV	C14-C13-N2	2.04	120.15	115.96
2	B	444	NOV	O5-C28-C27	2.38	113.35	108.17
2	A	400	NOV	O9-C8-C9	2.64	121.96	116.60
2	A	400	NOV	O1-C27-C28	2.64	115.34	109.29
2	A	400	NOV	O5-C28-C29	2.65	113.61	107.70
2	A	400	NOV	C7-N2-C13	2.87	130.93	123.38
2	A	400	NOV	C1-O1-C27	3.04	119.95	114.26
2	A	400	NOV	C20-C16-C17	3.17	125.76	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	NOV	C14-C13-N2	3.20	122.52	115.96
2	B	444	NOV	O1-C27-C28	3.44	117.17	109.29
2	A	400	NOV	O7-C31-C27	3.45	111.37	107.48
2	B	444	NOV	O9-C8-C9	3.75	124.21	116.60
2	B	444	NOV	O7-C31-C27	4.72	112.80	107.48
2	A	400	NOV	O5-C28-C27	6.22	121.73	108.17
2	A	400	NOV	C28-O5-C12	6.75	126.14	116.96
2	B	444	NOV	C28-O5-C12	9.85	130.35	116.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NOV	5	0
2	B	444	NOV	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	384/390 (98%)	0.21	34 (8%)	12	17	7, 23, 49, 60	0
1	B	384/390 (98%)	0.31	30 (7%)	16	22	6, 23, 49, 58	0
All	All	768/780 (98%)	0.26	64 (8%)	14	20	6, 23, 49, 60	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	THR	6.7
1	A	335	GLN	6.4
1	A	306	LYS	6.3
1	A	262	TYR	5.3
1	B	161	ARG	5.3
1	B	308	PRO	5.0
1	B	231	GLU	4.9
1	B	307	GLY	4.8
1	B	210	HIS	4.6
1	B	305	GLU	4.4
1	B	337	LYS	4.4
1	B	311	THR	4.2
1	B	304	LYS	4.1
1	B	392	VAL	4.1
1	B	232	GLY	4.1
1	A	210	HIS	4.1
1	A	304	LYS	4.0
1	A	305	GLU	3.9
1	B	309	GLN	3.7
1	A	232	GLY	3.6
1	B	335	GLN	3.5
1	A	209	GLN	3.3
1	A	390	GLU	3.3
1	A	336	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	298	LYS	3.2
1	B	262	TYR	3.2
1	A	300	ALA	3.1
1	B	310	PRO	3.1
1	B	366	ARG	3.0
1	A	212	LYS	3.0
1	A	392	VAL	3.0
1	A	380	GLN	2.9
1	A	366	ARG	2.9
1	B	390	GLU	2.9
1	B	208	ARG	2.9
1	A	263	ASN	2.8
1	B	106	GLY	2.7
1	B	306	LYS	2.6
1	B	209	GLN	2.5
1	A	276	ARG	2.5
1	A	9	ALA	2.5
1	A	307	GLY	2.5
1	B	303	ASN	2.5
1	A	298	LYS	2.5
1	A	238	GLU	2.4
1	A	334	GLY	2.4
1	A	301	GLY	2.4
1	A	231	GLU	2.4
1	B	84	GLU	2.3
1	A	308	PRO	2.3
1	A	303	ASN	2.3
1	A	234	ASP	2.3
1	A	383	GLU	2.2
1	B	230	ALA	2.2
1	A	309	GLN	2.2
1	A	312	GLY	2.2
1	A	211	GLY	2.1
1	B	73	ASN	2.1
1	A	389	ARG	2.1
1	A	355	GLU	2.1
1	A	391	LEU	2.1
1	B	334	GLY	2.1
1	B	160	PRO	2.1
1	B	9	ALA	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
2	NOV	A	400	44/44	0.82	0.20	1.61	12,20,76,84	0
2	NOV	B	444	44/44	0.80	0.19	1.21	19,24,77,84	0
3	FMT	B	441	3/3	0.88	0.11	-1.23	33,33,33,34	0
3	FMT	A	401	3/3	0.91	0.11	-	36,36,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.