Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:22 PM GMT

PDB ID	:	5CA0
Title	:	Crystal structure of T2R-TTL-Lexibulin complex
Authors	:	Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on	:	2015-06-29
Resolution	:	2.50 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:

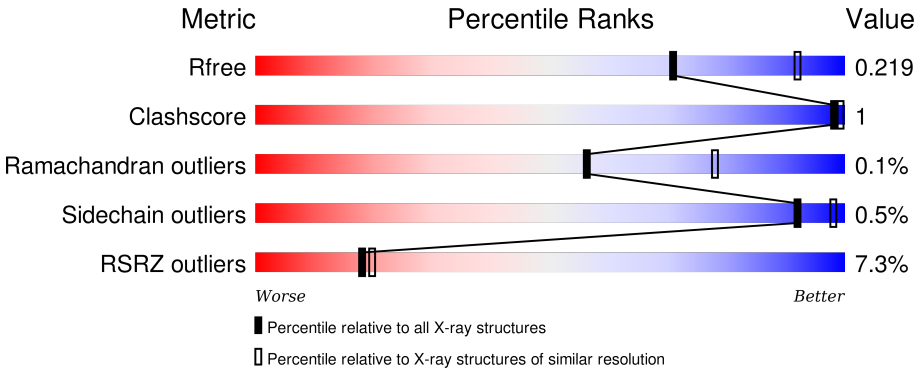
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	451	2% 96%
1	C	451	96%
2	B	445	5% 92%
2	D	445	12% 91% 5%
3	E	143	10% 85% 15%

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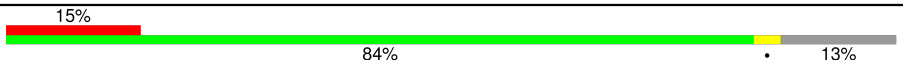
Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34509 atoms, of which 16844 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	426	Total	C	H	N	O	S	0	0	0
			6565	2104	3215	572	648	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

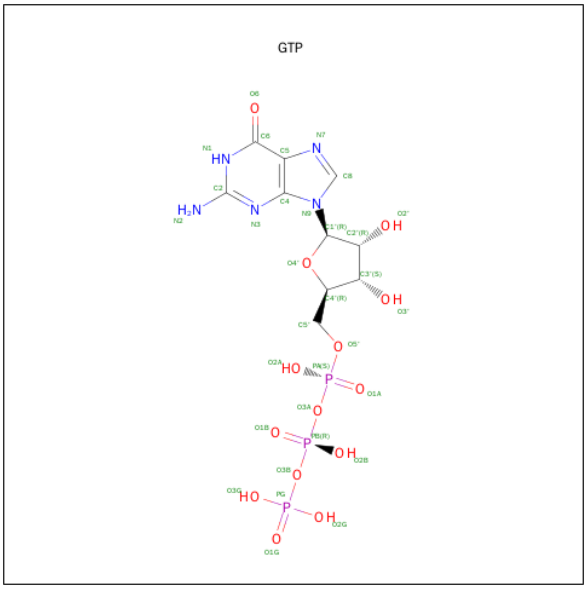
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

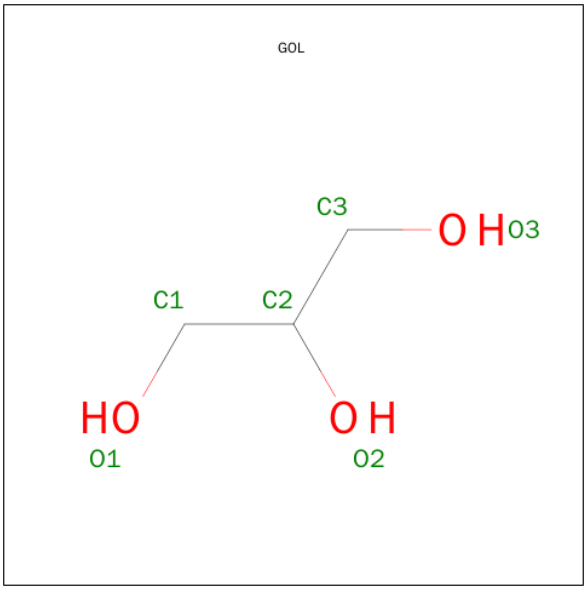
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

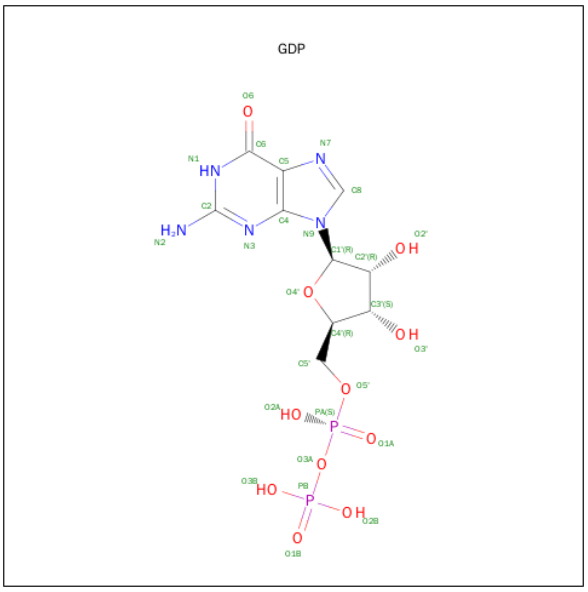
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



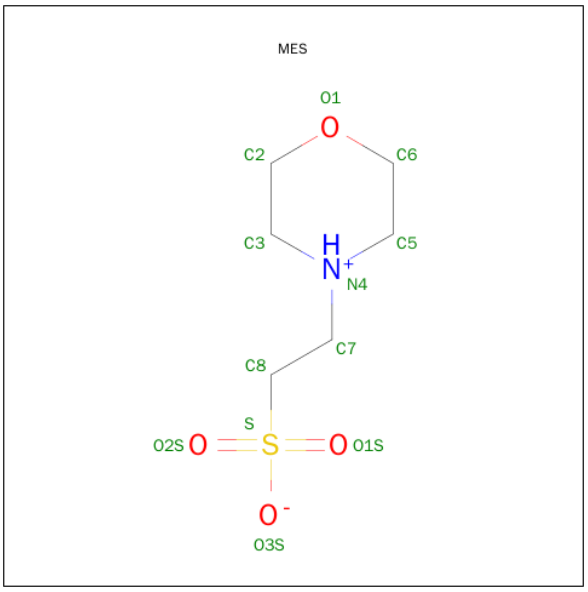
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 14 3 8 3	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



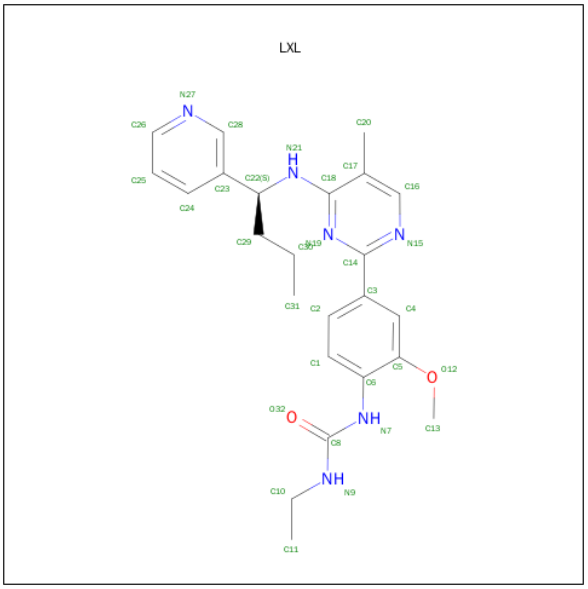
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
9	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



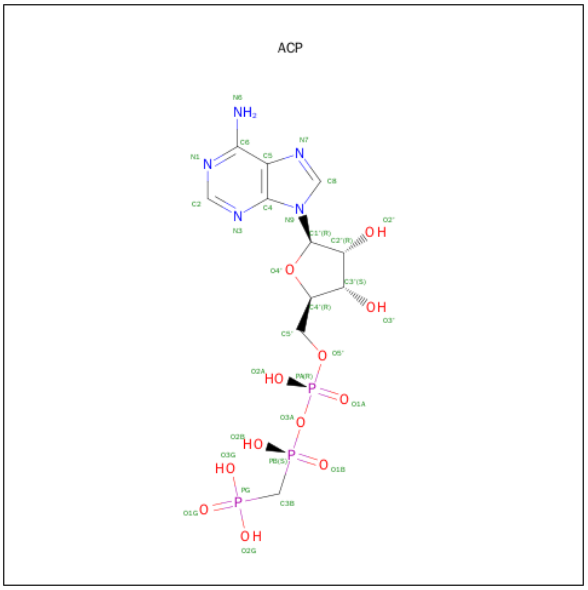
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 11 is 1-ethyl-3-[2-methoxy-4-(5-methyl-4-{[(1S)-1-(pyridin-3-yl)butyl]amino}pyrimidin-2-yl)phenyl]urea (three-letter code: LXL) (formula: $C_{24}H_{30}N_6O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			43	24	11	6	2		
11	D	1	Total	C	H	N	O	0	0
			43	24	11	6	2		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			35	11	4	5	12	3		

- Molecule 13 is water.

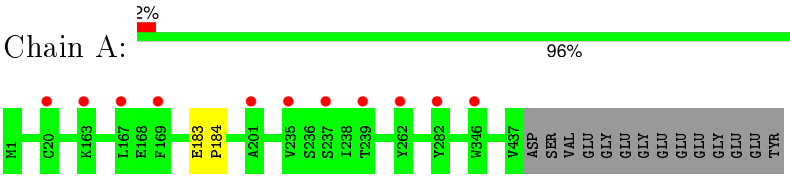
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	34	Total	O	0	0
			34	34		
13	B	29	Total	O	0	0
			29	29		
13	C	70	Total	O	0	0
			70	70		
13	D	17	Total	O	0	0
			17	17		
13	E	7	Total	O	0	0
			7	7		
13	F	14	Total	O	0	0
			14	14		

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.

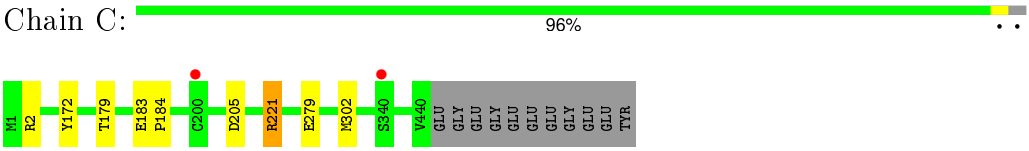
- Molecule 1: Tubulin alpha-1B chain

Chain A:



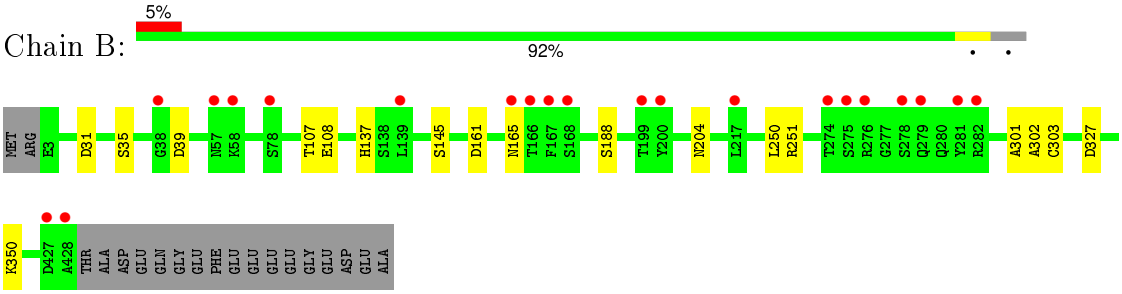
- Molecule 1: Tubulin alpha-1B chain

Chain C:



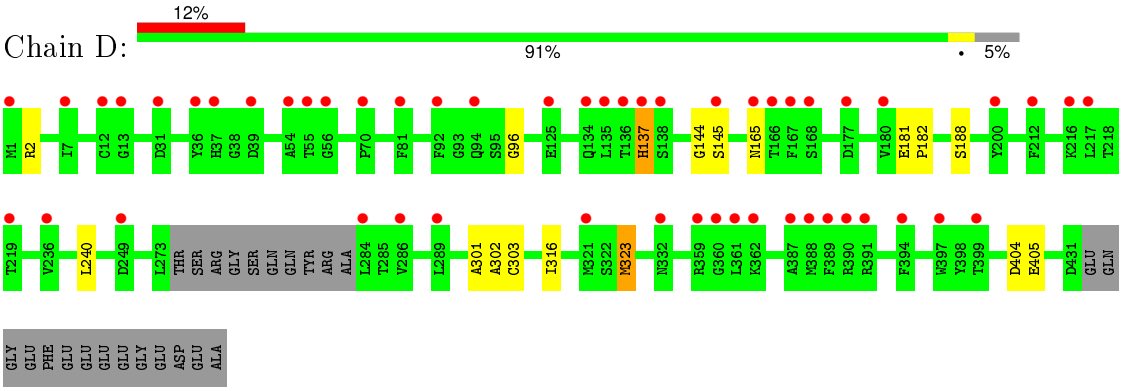
- Molecule 2: Uncharacterized protein

Chain B:



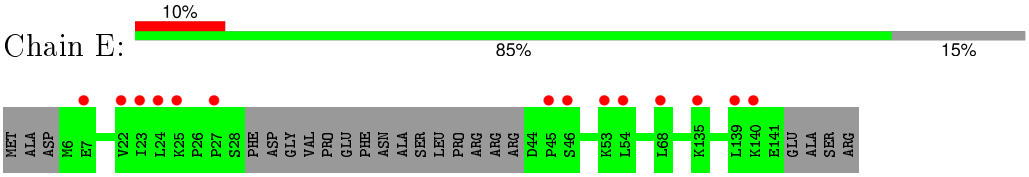
- Molecule 2: Uncharacterized protein

Chain D:



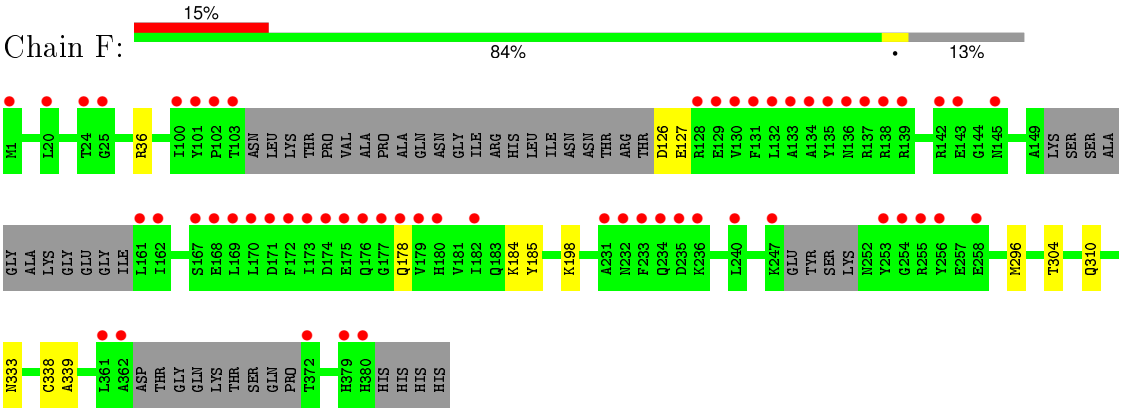
• Molecule 3: Stathmin-4

Chain E:



• Molecule 4: Uncharacterized protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.06Å 158.44Å 181.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.70 – 2.50 38.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.70-2.50) 99.2 (38.70-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.198 , 0.237 0.215 , 0.219	Depositor DCC
R_{free} test set	5180 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 104339 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34509	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: GDP, GOL, MG, CA, GTP, ACP, MES, LXL

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	0.21	0/3494	0.37	0/4743
1	C	0.21	0/3515	0.37	0/4772
2	B	0.22	0/3425	0.36	0/4640
2	D	0.22	0/3382	0.37	0/4581
3	E	0.21	0/1008	0.31	0/1337
4	F	0.21	0/2806	0.35	0/3791
All	All	0.21	0/17630	0.36	0/23864

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	3416	3317	3330	1	0
1	C	3437	3335	3348	5	0
2	B	3350	3215	3225	10	0
2	D	3309	3179	3189	10	0
3	E	1000	1014	1018	0	0
4	F	2744	2698	2709	8	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	28	10	12	1	0
9	D	28	10	12	0	0
10	B	12	12	12	0	0
11	B	32	11	30	3	0
11	D	32	11	30	5	0
12	F	31	4	14	2	0
13	A	34	0	0	0	0
13	B	29	0	0	0	0
13	C	70	0	0	0	0
13	D	17	0	0	0	0
13	E	7	0	0	0	0
13	F	14	0	0	1	0
All	All	17665	16844	16961	34	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 1.

All (34) 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)
12:F:401:ACP:H8	12:F:401:ACP:H5'1	1.61	0.82
2:B:250:LEU:HD21	11:B:504:LXL:H2	1.76	0.68
4:F:184:LYS:NZ	4:F:185:TYR:O	2.29	0.65
2:D:316:ILE:HD11	11:D:502:LXL:H9	1.85	0.59
4:F:304:THR:O	4:F:310:GLN:NE2	2.35	0.59
2:B:250:LEU:CD2	11:B:504:LXL:H2	2.34	0.58
4:F:36:ARG:NH2	13:F:501:HOH:O	2.37	0.56
1:C:221:ARG:NE	2:D:323:MET:SD	2.78	0.56
2:D:404:ASP:OD1	2:D:405:GLU:N	2.40	0.55
4:F:126:ASP:OD1	4:F:127:GLU:N	2.40	0.54
2:D:137:HIS:ND1	2:D:144:GLY:O	2.26	0.54
2:D:165:ASN:HD22	11:D:502:LXL:H1	1.76	0.50
2:B:301:ALA:O	2:B:303:CYS:N	2.46	0.48
2:B:145:SER:HG	2:B:188:SER:HG	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:ALA:O	2:D:303:CYS:N	2.47	0.48
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.47	0.47
4:F:178:GLN:OE1	4:F:178:GLN:N	2.46	0.47
1:C:279:GLU:OE1	1:C:279:GLU:N	2.46	0.46
2:D:181:GLU:N	2:D:182:PRO:HD2	2.31	0.45
2:D:145:SER:OG	2:D:188:SER:OG	2.33	0.45
2:B:39:ASP:OD1	2:B:39:ASP:N	2.48	0.45
4:F:333:ASN:ND2	12:F:401:ACP:O1G	2.44	0.44
2:B:165:ASN:HD22	11:B:504:LXL:H1	1.83	0.44
2:D:316:ILE:CD1	11:D:502:LXL:H9	2.47	0.43
2:B:31:ASP:OD1	2:B:35:SER:N	2.51	0.43
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.43
1:C:179:THR:O	11:D:502:LXL:H15	2.19	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.42
2:B:161:ASP:O	2:B:251:ARG:NH2	2.54	0.41
2:D:240:LEU:HD11	11:D:502:LXL:H2	2.03	0.41
2:B:107:THR:OG1	2:B:108:GLU:N	2.53	0.41
4:F:338:CYS:SG	4:F:339:ALA:N	2.94	0.41
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.03	0.41
2:B:204:ASN:OD1	9:B:501:GDP:O2'	2.37	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	435/451 (96%)	422 (97%)	13 (3%)	0	100	100
1	C	438/451 (97%)	431 (98%)	7 (2%)	0	100	100
2	B	424/445 (95%)	410 (97%)	13 (3%)	1 (0%)	52	75
2	D	417/445 (94%)	406 (97%)	9 (2%)	2 (0%)	34	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100 100
4	F	324/384 (84%)	315 (97%)	9 (3%)	0	100 100
All	All	2155/2319 (93%)	2099 (97%)	53 (2%)	3 (0%)	56 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	96	GLY
2	B	302	ALA
2	D	302	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	368/379 (97%)	368 (100%)	0	100 100
1	C	371/379 (98%)	368 (99%)	3 (1%)	86 96
2	B	368/383 (96%)	365 (99%)	3 (1%)	86 96
2	D	364/383 (95%)	361 (99%)	3 (1%)	86 96
3	E	109/127 (86%)	109 (100%)	0	100 100
4	F	301/342 (88%)	300 (100%)	1 (0%)	94 99
All	All	1881/1993 (94%)	1871 (100%)	10 (0%)	92 98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	327	ASP
2	B	350	LYS
1	C	2	ARG
1	C	221	ARG
1	C	302	MET
2	D	2	ARG

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Mol	Chain	Res	Type
2	D	137	HIS
2	D	323	MET
4	F	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	165	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

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.07	1 (3%)	26,54,54	0.83	0
8	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.22	0
9	GDP	B	501	6	24,30,30	1.40	4 (16%)	23,47,47	0.89	0
10	MES	B	503	-	12,12,12	1.92	1 (8%)	15,16,16	1.83	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	LXL	B	504	-	33,34,34	2.27	7 (21%)	38,45,45	2.37	11 (28%)
5	GTP	C	501	6	26,34,34	1.07	1 (3%)	26,54,54	0.83	0
9	GDP	D	501	-	24,30,30	1.40	4 (16%)	23,47,47	0.84	0
11	LXL	D	502	-	33,34,34	2.31	7 (21%)	38,45,45	2.27	11 (28%)
12	ACP	F	401	-	29,33,33	1.63	5 (17%)	29,52,52	1.73	6 (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
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	LXL	B	504	-	-	0/24/24/24	0/3/3/3
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3
11	LXL	D	502	-	-	0/24/24/24	0/3/3/3
12	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	LXL	C23-C22	-9.10	1.39	1.52
11	B	504	LXL	C23-C22	-8.76	1.39	1.52
10	B	503	MES	C8-S	-6.28	1.66	1.78
11	B	504	LXL	C20-C17	-5.97	1.39	1.51
11	D	502	LXL	C20-C17	-5.84	1.39	1.51
11	D	502	LXL	C6-N7	-4.41	1.33	1.41
11	B	504	LXL	C6-N7	-4.08	1.34	1.41
11	D	502	LXL	C3-C14	-3.51	1.39	1.48
11	B	504	LXL	C3-C14	-3.39	1.39	1.48
12	F	401	ACP	PG-O2G	-3.28	1.46	1.54
12	F	401	ACP	C2'-C1'	-2.28	1.50	1.53
12	F	401	ACP	C2'-C3'	-2.17	1.47	1.53
12	F	401	ACP	C4-N3	-2.09	1.32	1.35
9	B	501	GDP	C2-N3	2.09	1.36	1.33
11	B	504	LXL	C26-N27	2.23	1.40	1.33
11	D	502	LXL	C26-N27	2.25	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C2-N3	2.31	1.36	1.33
9	B	501	GDP	C2-N2	2.45	1.36	1.32
9	D	501	GDP	C2-N2	2.46	1.36	1.32
11	D	502	LXL	C28-N27	2.68	1.40	1.34
11	B	504	LXL	C28-N27	2.81	1.40	1.34
11	D	502	LXL	C16-N15	2.92	1.40	1.34
9	B	501	GDP	C5-C4	2.94	1.47	1.40
9	D	501	GDP	C5-C4	3.01	1.47	1.40
11	B	504	LXL	C16-N15	3.15	1.41	1.34
9	D	501	GDP	C6-C5	3.90	1.48	1.40
9	B	501	GDP	C6-C5	3.92	1.48	1.40
5	C	501	GTP	C2-N3	4.07	1.38	1.33
5	A	501	GTP	C2-N3	4.15	1.38	1.33
12	F	401	ACP	PG-O1G	4.70	1.60	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	502	LXL	C17-C16-N15	-8.34	118.84	125.33
11	B	504	LXL	C17-C16-N15	-7.84	119.22	125.33
11	B	504	LXL	C13-O12-C5	-6.01	108.75	117.53
12	F	401	ACP	N3-C2-N1	-5.31	124.70	128.87
11	B	504	LXL	N15-C14-N19	-5.04	120.82	125.35
11	D	502	LXL	N15-C14-N19	-4.45	121.35	125.35
12	F	401	ACP	O2'-C2'-C3'	-3.65	100.07	111.86
11	D	502	LXL	O32-C8-N7	-3.20	118.69	123.59
11	B	504	LXL	O32-C8-N7	-2.80	119.31	123.59
11	D	502	LXL	C23-C22-N21	-2.78	108.95	113.62
11	D	502	LXL	C23-C28-N27	-2.77	119.79	124.21
11	B	504	LXL	C23-C28-N27	-2.65	119.98	124.21
12	F	401	ACP	O4'-C1'-N9	-2.54	103.31	108.11
11	B	504	LXL	C23-C22-N21	-2.42	109.55	113.62
12	F	401	ACP	O3'-C3'-C2'	-2.41	104.08	111.86
12	F	401	ACP	C5'-C4'-C3'	-2.04	107.32	115.20
11	B	504	LXL	C6-N7-C8	-2.03	121.31	125.62
11	D	502	LXL	C13-O12-C5	-2.02	114.57	117.53
11	D	502	LXL	C2-C3-C4	2.30	121.08	118.17
12	F	401	ACP	O3G-PG-C3B	2.41	111.85	106.13
11	D	502	LXL	C16-N15-C14	2.77	119.65	116.10
11	B	504	LXL	C16-N15-C14	2.86	119.77	116.10
11	D	502	LXL	C3-C14-N15	3.02	120.73	117.31
11	B	504	LXL	C24-C23-C28	3.07	120.13	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	504	LXL	C3-C14-N15	3.11	120.83	117.31
11	D	502	LXL	C24-C23-C28	3.41	120.51	116.76
10	B	503	MES	C7-N4-C5	3.45	118.77	111.25
11	B	504	LXL	N7-C8-N9	4.26	120.86	113.91
11	D	502	LXL	N7-C8-N9	4.73	121.62	113.91
10	B	503	MES	C5-N4-C3	5.00	120.06	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	GDP	1	0
11	B	504	LXL	3	0
11	D	502	LXL	5	0
12	F	401	ACP	2	0

5.7 Other polymers

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	437/451 (96%)	0.21	11 (2%) 61 65	42, 61, 91, 115	0
1	C	440/451 (97%)	0.02	2 (0%) 91 92	38, 53, 82, 113	0
2	B	426/445 (95%)	0.33	21 (4%) 33 38	40, 61, 97, 142	0
2	D	421/445 (94%)	0.63	52 (12%) 5 5	45, 76, 110, 134	0
3	E	121/143 (84%)	0.48	14 (11%) 6 6	49, 77, 107, 121	0
4	F	334/384 (86%)	0.84	58 (17%) 2 2	52, 84, 135, 161	0
All	All	2179/2319 (93%)	0.39	158 (7%) 18 20	38, 66, 111, 161	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	7.5
4	F	169	LEU	6.7
4	F	176	GLN	6.5
4	F	172	PHE	6.4
4	F	132	LEU	6.2
4	F	161	LEU	6.2
4	F	178	GLN	6.1
4	F	138	ARG	5.9
2	B	57	ASN	5.7
2	B	428	ALA	5.7
4	F	142	ARG	5.6
4	F	177	GLY	5.5
4	F	103	THR	5.3
4	F	175	GLU	5.3
4	F	100	ILE	5.0
4	F	233	PHE	4.9
4	F	135	TYR	4.9
4	F	101	TYR	4.8
4	F	234	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	102	PRO	4.8
3	E	24	LEU	4.7
4	F	170	LEU	4.5
4	F	361	LEU	4.5
2	D	390	ARG	4.4
2	D	55	THR	4.4
4	F	236	LYS	4.4
2	D	394	PHE	4.4
4	F	182	ILE	4.2
3	E	139	LEU	4.1
4	F	137	ARG	4.1
4	F	145	ASN	4.1
2	D	391	ARG	4.0
2	B	279	GLN	3.9
4	F	372	THR	3.9
4	F	20	LEU	3.9
4	F	134	ALA	3.8
4	F	168	GLU	3.8
2	D	37	HIS	3.8
4	F	139	ARG	3.8
4	F	231	ALA	3.7
2	B	274	THR	3.7
2	B	275	SER	3.6
4	F	136	ASN	3.6
4	F	232	ASN	3.6
4	F	131	PHE	3.6
2	D	137	HIS	3.6
4	F	133	ALA	3.6
4	F	180	HIS	3.5
2	D	362	LYS	3.5
2	D	168	SER	3.4
4	F	167	SER	3.4
3	E	25	LYS	3.4
2	B	58	LYS	3.3
4	F	162	ILE	3.3
2	D	219	THR	3.2
2	D	166	THR	3.2
3	E	135	LYS	3.1
2	B	276	ARG	3.1
3	E	46	SER	3.1
2	D	136	THR	3.1
1	C	340	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	278	SER	3.1
3	E	27	PRO	3.1
2	D	200	TYR	3.0
2	B	168	SER	3.0
4	F	380	HIS	3.0
2	D	217	LEU	3.0
2	D	94	GLN	3.0
2	D	397	TRP	2.9
2	D	1	MET	2.9
4	F	174	ASP	2.9
2	D	92	PHE	2.9
1	A	282	TYR	2.9
2	D	216	LYS	2.9
4	F	253	TYR	2.9
4	F	128	ARG	2.9
4	F	362	ALA	2.9
2	D	167	PHE	2.8
2	B	200	TYR	2.8
2	B	166	THR	2.8
4	F	130	VAL	2.8
2	D	125	GLU	2.8
1	A	201	ALA	2.8
2	B	167	PHE	2.7
2	D	177	ASP	2.7
1	A	346	TRP	2.7
4	F	235	ASP	2.7
1	A	239	THR	2.7
4	F	24	THR	2.6
3	E	23	ILE	2.5
2	D	249	ASP	2.5
2	D	387	ALA	2.5
2	D	13	GLY	2.5
2	D	165	ASN	2.5
2	D	54	ALA	2.5
2	B	165	ASN	2.5
2	B	78	SER	2.5
1	C	200	CYS	2.4
4	F	179	VAL	2.4
1	A	235	VAL	2.4
2	D	180	VAL	2.4
2	D	236	VAL	2.4
3	E	7	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	427	ASP	2.4
3	E	54	LEU	2.4
2	D	7	ILE	2.3
2	D	389	PHE	2.3
2	B	38	GLY	2.3
2	D	31	ASP	2.3
4	F	171	ASP	2.3
3	E	22	VAL	2.3
2	D	286	VAL	2.3
1	A	20	CYS	2.3
2	D	56	GLY	2.2
2	D	321	MET	2.2
2	D	212	PHE	2.2
4	F	143	GLU	2.2
4	F	379	HIS	2.2
1	A	262	TYR	2.2
4	F	255	ARG	2.2
4	F	129	GLU	2.2
2	D	12	CYS	2.2
4	F	1	MET	2.2
4	F	240	LEU	2.2
2	D	145	SER	2.2
3	E	53	LYS	2.2
4	F	247	LYS	2.2
4	F	254	GLY	2.2
2	D	36	TYR	2.2
2	D	135	LEU	2.2
2	D	361	LEU	2.2
1	A	237	SER	2.2
2	D	134	GLN	2.1
2	D	399	THR	2.1
2	D	81	PHE	2.1
2	B	281	TYR	2.1
4	F	256	TYR	2.1
2	B	217	LEU	2.1
3	E	140	LYS	2.1
2	D	70	PRO	2.1
3	E	45	PRO	2.1
2	D	332	ASN	2.1
1	A	163	LYS	2.1
2	D	39	ASP	2.1
2	B	282	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	199	THR	2.0
1	A	169	PHE	2.0
2	D	284	LEU	2.0
2	D	359	ARG	2.0
2	D	388	MET	2.0
2	D	138	SER	2.0
2	B	139	LEU	2.0
3	E	68	LEU	2.0
4	F	25	GLY	2.0
2	D	360	GLY	2.0
1	A	167	LEU	2.0
2	D	289	LEU	2.0
4	F	258	GLU	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
9	GDP	B	501	28/28	0.94	0.26	1.87	45,59,90,117	0
6	MG	C	502	1/1	0.98	0.22	1.80	46,46,46,46	0
11	LXL	B	504	32/32	0.93	0.28	1.33	39,54,80,99	0
6	MG	A	502	1/1	0.97	0.20	1.30	48,48,48,48	0
9	GDP	D	501	28/28	0.86	0.25	0.86	50,75,117,162	0
11	LXL	D	502	32/32	0.90	0.26	0.71	34,63,93,103	43
5	GTP	A	501	32/32	0.97	0.20	0.64	39,53,74,75	0
5	GTP	C	501	32/32	0.97	0.20	0.53	37,51,66,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	MES	B	503	12/12	0.96	0.19	0.19	53,72,91,97	0
8	GOL	A	504	6/6	0.87	0.15	0.13	64,82,98,117	0
12	ACP	F	401	31/31	0.93	0.19	-0.74	76,103,149,175	0
7	CA	A	503	1/1	0.85	0.08	-1.30	81,81,81,81	0
7	CA	C	503	1/1	0.92	0.06	-3.17	71,71,71,71	0
6	MG	B	502	1/1	0.94	0.43	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.