



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2016 – 03:39 PM EDT

PDB ID : 5LP6
Title : Crystal structure of Tubulin-Stathmin-TTL-Thiocolchicine Complex
Authors : Marangon, J.; Christodoulou, M.; Casagrande, F.; Tiana, G.; Dalla Via, L.; Aliverti, A.; Passarella, D.; Cappelletti, G.; Ricagno, S.
Deposited on : 2016-08-11
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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-20027939

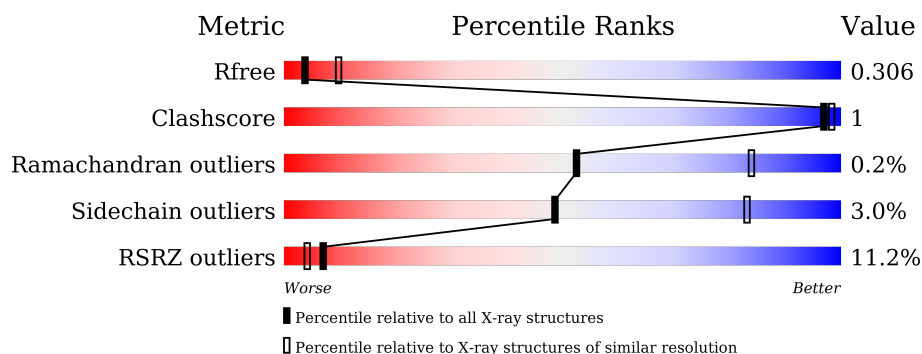
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
2	B	445	<div> <div>4%</div> <div>92%</div> <div>• 5%</div> </div>
2	D	445	<div> <div>9%</div> <div>91%</div> <div>• 5%</div> </div>
3	C	440	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
4	E	143	<div> <div>8%</div> <div>80%</div> <div>• 15%</div> </div>
5	F	384	<div> <div>34%</div> <div>83%</div> <div>5%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	71P	B	504	-	-	-	X
12	CA	C	503	-	-	-	X
7	MG	A	502	-	-	-	X
7	MG	A	506	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17547 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3318	2085	566	640	27			
2	D	421	Total	C	N	O	S	0	0	0
			3308	2079	562	641	26			

- Molecule 3 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 4 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

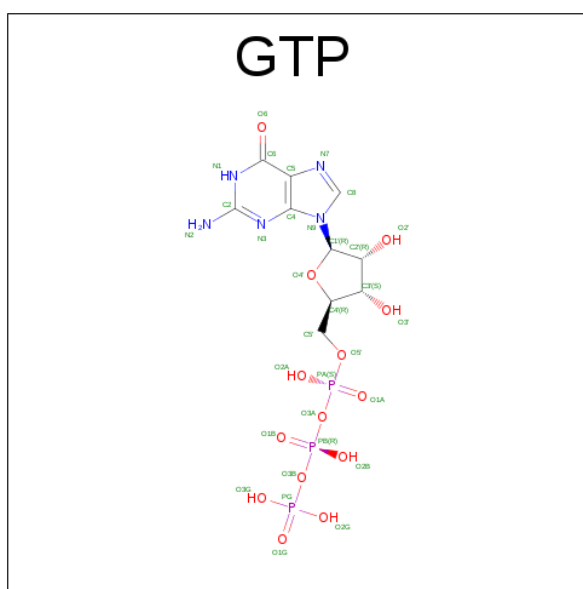
- Molecule 5 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	340	Total	C	N	O	S	0	0	0
			2794	1795	476	509	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 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
6	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Mg	0	0
			3	3		

Continued on next page...

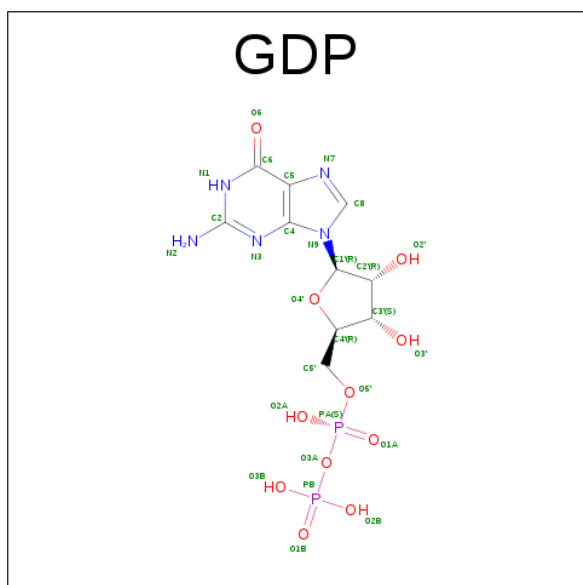
Continued from previous page...

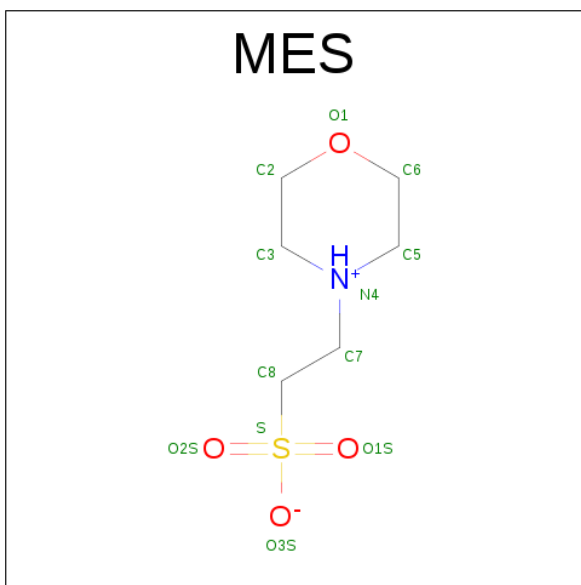
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Mg	0	0
			4	4		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

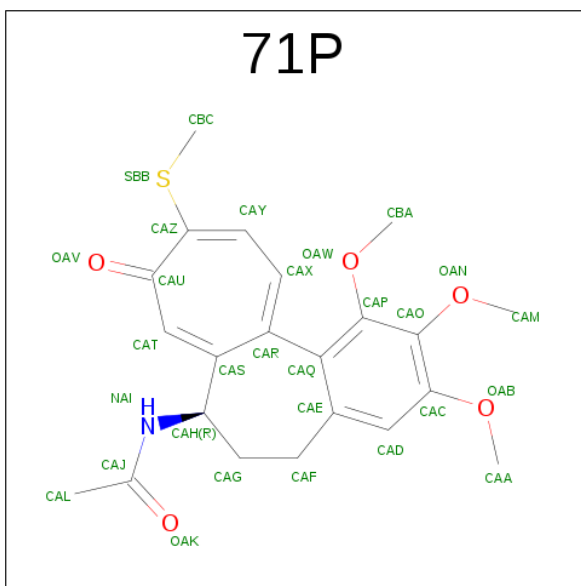
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





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

- Molecule 11 is {N}-[(7 {R})-1,2,3-trimethoxy-10-methylsulfanyl-9-oxidanylidene-6,7-dihydro-5 {H}-benzo[a]heptalen-7-yl]ethanamide (three-letter code: 71P) (formula: C₂₂H₂₅NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Ca 1 1	0	0

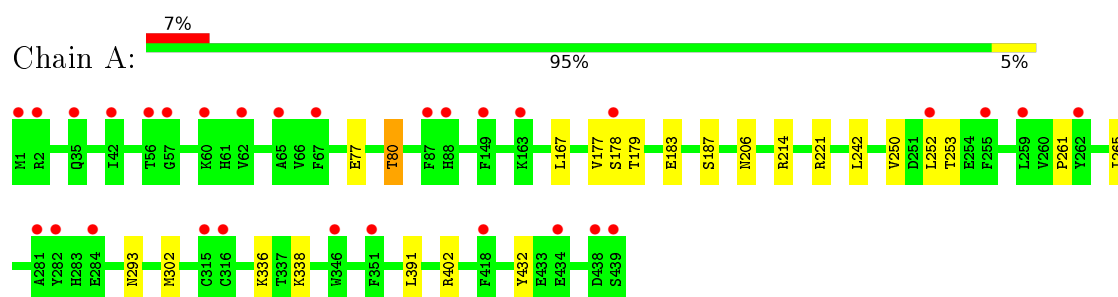
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	21	Total O 21 21	0	0
13	B	16	Total O 16 16	0	0
13	C	35	Total O 35 35	0	0
13	D	11	Total O 11 11	0	0
13	E	1	Total O 1 1	0	0
13	F	5	Total O 5 5	0	0

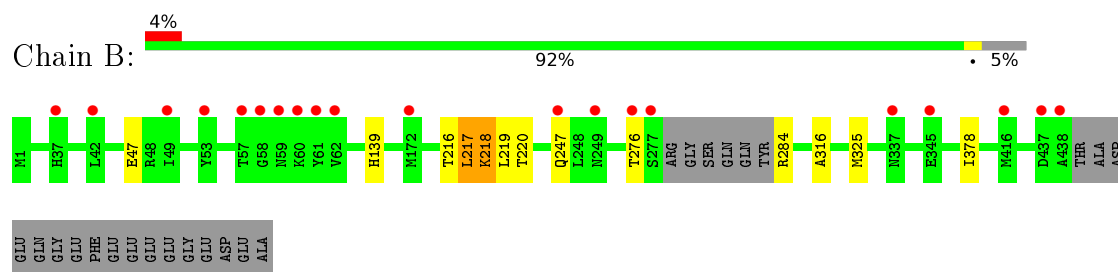
3 Residue-property plots

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.

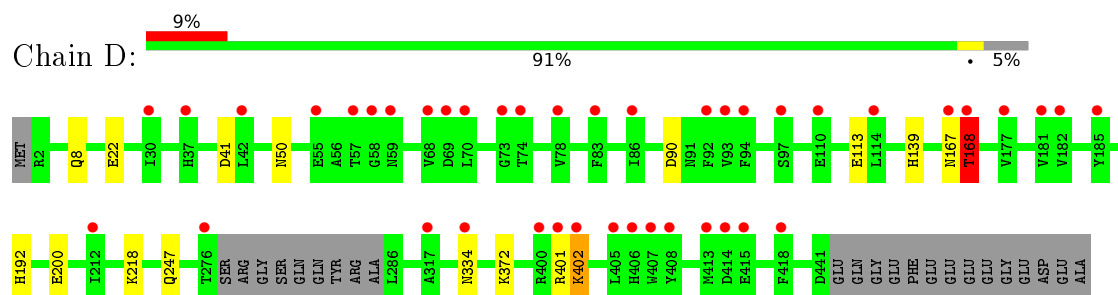
- Molecule 1: Tubulin alpha-1B chain



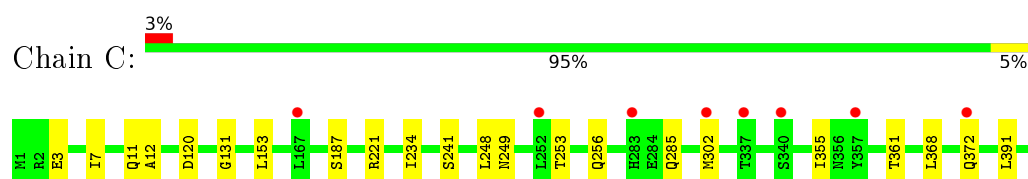
- Molecule 2: Tubulin beta-2B chain



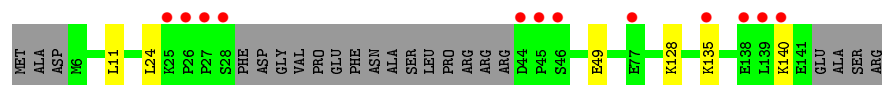
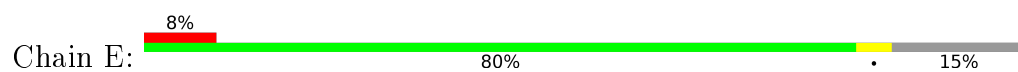
- Molecule 2: Tubulin beta-2B chain



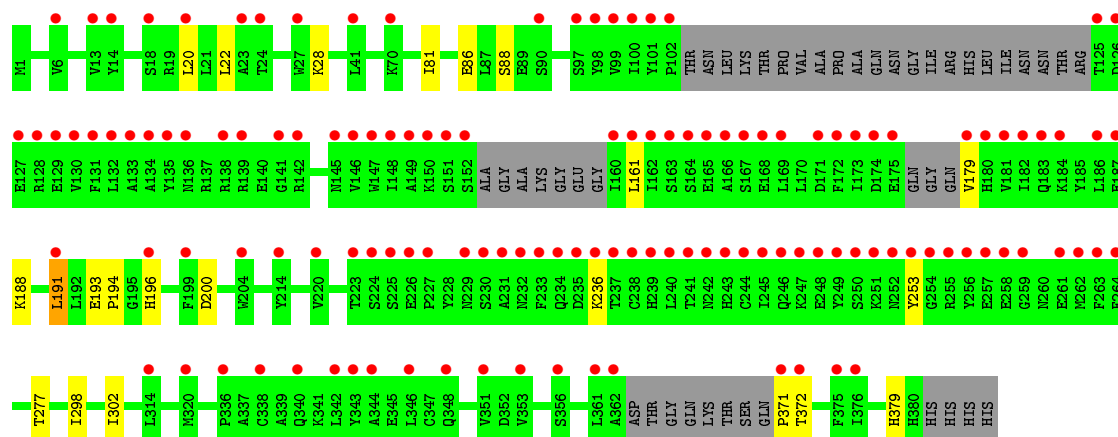
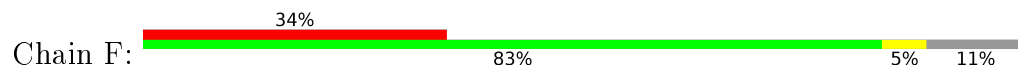
- Molecule 3: Tubulin alpha-1B chain



- Molecule 4: Stathmin-4



• Molecule 5: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.62Å 155.28Å 180.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.85 – 2.90 58.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.85-2.90) 99.8 (58.85-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.273 , 0.305 0.273 , 0.306	Depositor DCC
R_{free} test set	3307 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17547	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 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CL, CA, 71P, GTP, MES

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	0.38	0/3508	0.57	0/4762
2	B	0.36	0/3389	0.57	0/4586
2	D	0.37	0/3379	0.56	0/4575
3	C	0.35	0/3515	0.57	0/4772
4	E	0.35	0/1008	0.52	0/1337
5	F	0.39	0/2858	0.58	0/3860
All	All	0.37	0/17657	0.57	0/23892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3340	14	0
2	B	3318	0	3201	9	0
2	D	3308	0	3182	3	0
3	C	3437	0	3348	10	0
4	E	1000	0	1018	0	0
5	F	2794	0	2765	8	0
6	A	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	32	0	12	0	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	12	0	13	0	0
11	B	29	0	0	2	0
12	C	1	0	0	0	0
13	A	21	0	0	0	0
13	B	16	0	0	0	0
13	C	35	0	0	1	0
13	D	11	0	0	0	0
13	E	1	0	0	0	0
13	F	5	0	0	0	0
All	All	17547	0	16915	44	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 (44) 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)
2:B:216:THR:O	2:B:218:LYS:N	1.75	1.17
1:A:177:VAL:O	1:A:178:SER:OG	1.59	1.17
5:F:191:LEU:HG	5:F:196:HIS:CE1	2.13	0.82
1:A:177:VAL:C	1:A:178:SER:HG	1.83	0.77
1:A:177:VAL:O	1:A:178:SER:CB	2.42	0.68
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.82	0.61
2:B:218:LYS:C	2:B:219:LEU:HD23	2.21	0.61
1:A:179:THR:HB	1:A:183:GLU:CD	2.25	0.57
3:C:3:GLU:OE1	3:C:131:GLY:O	2.24	0.56
3:C:12:ALA:N	13:C:601:HOH:O	2.40	0.54
2:B:216:THR:O	2:B:218:LYS:CA	2.56	0.52
1:A:179:THR:HB	1:A:183:GLU:OE2	2.12	0.51
1:A:177:VAL:CG2	1:A:206:ASN:HB3	2.41	0.50
3:C:7:ILE:HG21	3:C:153:LEU:HD21	1.94	0.50
3:C:248:LEU:HD13	3:C:355:ILE:HD12	1.93	0.50
3:C:187:SER:HB3	3:C:391:LEU:HD21	1.94	0.49
2:B:216:THR:O	2:B:217:LEU:C	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.95	0.49
11:B:504:71P:CAX	11:B:504:71P:OAW	2.60	0.49
1:A:177:VAL:HG21	1:A:206:ASN:CB	2.41	0.49
1:A:177:VAL:HG11	6:A:501:GTP:O2'	2.14	0.47
5:F:191:LEU:HG	5:F:196:HIS:ND1	2.29	0.47
5:F:161:LEU:HA	5:F:236:LYS:HE2	1.97	0.47
2:D:167:ASN:O	2:D:168:THR:HG22	2.15	0.47
2:D:401:ARG:C	2:D:402:LYS:HG2	2.36	0.46
2:B:219:LEU:HD23	2:B:219:LEU:N	2.30	0.46
1:A:242:LEU:HD11	1:A:252:LEU:HD21	1.97	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.45
3:C:234:ILE:HG21	3:C:302:MET:SD	2.57	0.45
2:B:216:THR:C	2:B:218:LYS:N	2.61	0.44
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.00	0.44
3:C:11:GLN:O	3:C:12:ALA:HB3	2.18	0.44
5:F:298:ILE:HD12	5:F:302:ILE:HD13	1.99	0.44
3:C:11:GLN:HE22	2:D:247:GLN:HE22	1.66	0.43
5:F:371:PRO:HA	5:F:372:THR:HB	1.99	0.43
2:B:216:THR:HG22	2:B:217:LEU:H	1.83	0.43
2:B:316:ALA:HB1	11:B:504:71P:CBA	2.49	0.43
3:C:241:SER:HA	3:C:249:ASN:HD21	1.83	0.43
5:F:81:ILE:O	5:F:88:SER:HB3	2.18	0.42
5:F:193:GLU:HA	5:F:194:PRO:C	2.39	0.42
5:F:191:LEU:HB3	5:F:196:HIS:HA	2.02	0.41
3:C:234:ILE:HD13	3:C:302:MET:HE3	2.02	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
1:A:77:GLU:HA	1:A:80:THR:HG22	2.02	0.41

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	437/439 (100%)	423 (97%)	13 (3%)	1 (0%)	52	84
2	B	414/445 (93%)	400 (97%)	12 (3%)	2 (0%)	34	71
2	D	413/445 (93%)	400 (97%)	12 (3%)	1 (0%)	52	84
3	C	438/440 (100%)	428 (98%)	10 (2%)	0	100	100
4	E	117/143 (82%)	114 (97%)	3 (3%)	0	100	100
5	F	330/384 (86%)	310 (94%)	20 (6%)	0	100	100
All	All	2149/2296 (94%)	2075 (97%)	70 (3%)	4 (0%)	52	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	LEU
2	B	218	LYS
2	D	168	THR
1	A	261	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	370/370 (100%)	360 (97%)	10 (3%)	52	84
2	B	365/383 (95%)	358 (98%)	7 (2%)	65	89
2	D	364/383 (95%)	350 (96%)	14 (4%)	40	76
3	C	371/371 (100%)	363 (98%)	8 (2%)	60	88
4	E	109/127 (86%)	103 (94%)	6 (6%)	27	61
5	F	308/342 (90%)	297 (96%)	11 (4%)	42	78
All	All	1887/1976 (96%)	1831 (97%)	56 (3%)	48	83

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	ARG
1	A	221	ARG
1	A	250	VAL
1	A	253	THR
1	A	293	ASN
1	A	302	MET
1	A	336	LYS
1	A	338	LYS
1	A	402	ARG
2	B	47	GLU
2	B	139	HIS
2	B	220	THR
2	B	247	GLN
2	B	276	THR
2	B	284	ARG
2	B	325	MET
3	C	120	ASP
3	C	221	ARG
3	C	253	THR
3	C	256	GLN
3	C	285	GLN
3	C	361	THR
3	C	368	LEU
3	C	372	GLN
2	D	8	GLN
2	D	22	GLU
2	D	41	ASP
2	D	50	ASN
2	D	90	ASP
2	D	113	GLU
2	D	139	HIS
2	D	168	THR
2	D	192	HIS
2	D	200	GLU
2	D	218	LYS
2	D	334	ASN
2	D	372	LYS
2	D	402	LYS
4	E	11	LEU
4	E	24	LEU
4	E	49	GLU
4	E	128	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	135	LYS
4	E	140	LYS
5	F	20	LEU
5	F	22	LEU
5	F	28	LYS
5	F	86	GLU
5	F	179	VAL
5	F	188	LYS
5	F	191	LEU
5	F	200	ASP
5	F	253	TYR
5	F	277	THR
5	F	379	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	247	GLN
2	D	247	GLN
2	D	385	GLN
4	E	18	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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$
6	GTP	A	501	7	26,34,34	1.17	2 (7%)	29,54,54	1.87	5 (17%)
9	GDP	B	501	7	24,30,30	1.22	2 (8%)	26,47,47	1.94	4 (15%)
10	MES	B	503	-	12,12,12	2.20	1 (8%)	15,16,16	1.66	4 (26%)
11	71P	B	504	-	29,31,31	1.76	6 (20%)	27,44,44	3.25	12 (44%)
6	GTP	C	501	7	26,34,34	1.16	2 (7%)	29,54,54	1.86	5 (17%)
9	GDP	D	600	-	24,30,30	1.20	2 (8%)	26,47,47	2.00	5 (19%)

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
6	GTP	A	501	7	-	0/18/38/38	0/3/3/3
9	GDP	B	501	7	-	0/12/32/32	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	71P	B	504	-	-	1/10/25/25	0/3/3/3
6	GTP	C	501	7	-	0/18/38/38	0/3/3/3
9	GDP	D	600	-	-	0/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.29	1.66	1.77
11	B	504	71P	CAF-CAE	-4.96	1.41	1.51
11	B	504	71P	CAS-CAH	-4.50	1.43	1.52
11	B	504	71P	CAG-CAF	-3.22	1.43	1.53
11	B	504	71P	CAR-CAQ	-2.13	1.46	1.49
11	B	504	71P	CAQ-CAP	2.08	1.45	1.40
11	B	504	71P	CAH-NAI	3.07	1.51	1.46
6	C	501	GTP	C5-C4	3.13	1.47	1.40
9	D	600	GDP	C5-C4	3.14	1.47	1.40
6	A	501	GTP	C5-C4	3.17	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C5-C4	3.18	1.47	1.40
6	C	501	GTP	C6-C5	3.72	1.48	1.41
6	A	501	GTP	C6-C5	3.78	1.49	1.41
9	D	600	GDP	C6-C5	3.79	1.49	1.41
9	B	501	GDP	C6-C5	3.84	1.49	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	71P	CAF-CAE-CAD	-5.43	107.31	119.23
11	B	504	71P	CAP-CAQ-CAE	-4.49	112.58	118.16
6	A	501	GTP	C5-C6-N1	-4.23	118.00	123.52
9	D	600	GDP	C5-C6-N1	-4.19	118.04	123.52
9	B	501	GDP	C5-C6-N1	-4.14	118.11	123.52
6	C	501	GTP	C5-C6-N1	-4.14	118.11	123.52
9	D	600	GDP	N3-C2-N1	-3.93	122.22	127.56
9	B	501	GDP	N3-C2-N1	-3.88	122.28	127.56
11	B	504	71P	CBA-OAW-CAP	-3.73	104.87	114.82
9	D	600	GDP	C6-C5-C4	-3.71	116.62	120.86
6	A	501	GTP	N3-C2-N1	-3.69	122.53	127.56
6	C	501	GTP	N3-C2-N1	-3.68	122.55	127.56
6	C	501	GTP	C6-C5-C4	-3.66	116.68	120.86
11	B	504	71P	CAA-OAB-CAC	-3.65	112.20	117.53
6	A	501	GTP	C6-C5-C4	-3.64	116.70	120.86
9	B	501	GDP	C6-C5-C4	-3.54	116.82	120.86
11	B	504	71P	OAW-CAP-CAO	-3.32	112.53	120.38
9	D	600	GDP	C1'-N9-C4	-2.40	124.13	126.81
6	C	501	GTP	C1'-N9-C4	-2.22	124.33	126.81
6	A	501	GTP	C1'-N9-C4	-2.21	124.33	126.81
11	B	504	71P	OAK-CAJ-CAL	-2.14	118.13	122.07
10	B	503	MES	C5-N4-C3	2.02	113.39	108.87
11	B	504	71P	CAM-OAN-CAO	2.07	120.35	114.82
11	B	504	71P	OAK-CAJ-NAI	2.15	126.23	121.84
10	B	503	MES	O3S-S-C8	2.30	109.78	104.99
11	B	504	71P	OAW-CAP-CAQ	2.66	123.66	119.08
11	B	504	71P	CAR-CAQ-CAE	2.69	123.62	120.48
10	B	503	MES	O2S-S-C8	3.00	108.99	106.87
10	B	503	MES	O1S-S-C8	3.27	109.18	106.87
11	B	504	71P	CAG-CAH-NAI	5.17	119.39	110.03
6	C	501	GTP	C6-N1-C2	5.63	122.48	115.88
6	A	501	GTP	C6-N1-C2	5.75	122.62	115.88
9	B	501	GDP	C6-N1-C2	5.80	122.68	115.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	600	GDP	C6-N1-C2	5.92	122.82	115.88
11	B	504	71P	CAF-CAE-CAQ	11.04	130.25	119.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	504	71P	CAS-CAH-NAI-CAJ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	GTP	1	0
11	B	504	71P	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	360:PRO	C	369:ARG	N	3.14
1	B	42:LEU	C	45:GLN	N	3.11
1	D	42:LEU	C	45:GLN	N	3.03
1	D	360:PRO	C	369:ARG	N	2.87

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	439/439 (100%)	0.77	30 (6%)	20 14	64, 76, 84, 94	0
2	B	422/445 (94%)	0.80	20 (4%)	35 29	64, 76, 84, 92	1 (0%)
2	D	421/445 (94%)	0.83	42 (9%)	9 5	69, 77, 86, 93	5 (1%)
3	C	440/440 (100%)	0.71	11 (2%)	61 55	64, 75, 83, 88	0
4	E	121/143 (84%)	0.91	12 (9%)	9 5	71, 80, 86, 91	0
5	F	340/384 (88%)	1.80	129 (37%)	0 0	72, 79, 91, 99	0
All	All	2183/2296 (95%)	0.94	244 (11%)	7 4	64, 77, 87, 99	6 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	249	TYR	9.7
4	E	27	PRO	8.0
5	F	173	ILE	7.8
5	F	179	VAL	7.6
5	F	240	LEU	7.2
5	F	181	VAL	7.2
5	F	250	SER	6.9
5	F	100	ILE	6.7
5	F	130	VAL	6.5
5	F	131	PHE	6.4
5	F	231	ALA	6.1
1	A	439	SER	6.1
1	A	438	ASP	6.0
5	F	182	ILE	5.9
5	F	101	TYR	5.9
5	F	238	CYS	5.8
5	F	161	LEU	5.7
5	F	167	SER	5.6
5	F	248	GLU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	233	PHE	5.5
5	F	163	SER	5.5
5	F	134	ALA	5.5
5	F	251	LYS	5.4
5	F	256	TYR	5.3
5	F	232	ASN	5.2
5	F	253	TYR	5.0
5	F	239	HIS	5.0
5	F	224	SER	4.8
5	F	236	LYS	4.7
5	F	168	GLU	4.7
5	F	150	LYS	4.7
5	F	142	ARG	4.7
5	F	180	HIS	4.6
5	F	145	ASN	4.6
3	C	340	SER	4.6
5	F	149	ALA	4.5
5	F	225	SER	4.5
5	F	243	HIS	4.4
5	F	102	PRO	4.3
5	F	162	ILE	4.3
5	F	234	GLN	4.3
5	F	252	ASN	4.3
5	F	147	TRP	4.1
5	F	237	THR	4.1
5	F	244	CYS	4.1
5	F	196	HIS	4.1
5	F	139	ARG	4.1
5	F	128	ARG	4.0
2	D	401	ARG	4.0
2	B	61	TYR	4.0
5	F	174	ASP	4.0
1	A	346	TRP	4.0
1	A	1	MET	3.9
2	D	57	THR	3.9
5	F	255	ARG	3.9
5	F	241	THR	3.9
5	F	230	SER	3.9
5	F	169	LEU	3.9
5	F	132	LEU	3.8
5	F	136	ASN	3.8
5	F	371	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	182	VAL	3.8
5	F	254	GLY	3.8
5	F	245	ILE	3.8
4	E	26	PRO	3.7
1	A	281	ALA	3.7
5	F	171	ASP	3.7
5	F	138	ARG	3.7
5	F	165	GLU	3.7
3	C	302	MET	3.7
2	D	415	GLU	3.6
5	F	166	ALA	3.6
5	F	148	ILE	3.6
4	E	28	SER	3.6
2	B	276	THR	3.6
1	A	42	ILE	3.5
2	D	42	LEU	3.5
3	C	440	VAL	3.5
5	F	362	ALA	3.5
2	D	414	ASP	3.5
5	F	372	THR	3.5
2	B	42	LEU	3.5
5	F	183	GLN	3.4
5	F	235	ASP	3.4
5	F	129	GLU	3.4
2	B	57	THR	3.4
5	F	361	LEU	3.4
2	B	277	SER	3.4
2	B	249	ASN	3.4
2	B	337	ASN	3.4
5	F	263	PHE	3.3
5	F	172	PHE	3.3
5	F	343	TYR	3.3
4	E	135	LYS	3.3
1	A	262	TYR	3.3
2	D	181	VAL	3.2
5	F	242	ASN	3.2
5	F	246	GLN	3.2
2	D	406	HIS	3.2
5	F	99	VAL	3.2
2	B	437	ASP	3.2
2	D	177	VAL	3.2
1	A	60	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	20	LEU	3.1
2	B	247	GLN	3.1
2	D	37	HIS	3.1
5	F	247	LYS	3.1
5	F	164	SER	3.1
5	F	229	ASN	3.1
2	D	73	GLY	3.1
5	F	344	ALA	3.0
5	F	199	PHE	3.0
2	B	59	ASN	3.0
5	F	133	ALA	3.0
5	F	141	GLY	2.9
2	D	74	THR	2.9
4	E	77	GLU	2.9
5	F	262	MET	2.9
5	F	151	SER	2.9
5	F	175	GLU	2.9
5	F	214	TYR	2.9
4	E	45	PRO	2.9
2	D	400	ARG	2.9
2	D	94	PHE	2.9
5	F	6	VAL	2.9
5	F	160	ILE	2.9
2	D	68	VAL	2.9
5	F	261	GLU	2.8
1	A	57	GLY	2.8
2	B	172	MET	2.8
4	E	46	SER	2.8
5	F	127	GLU	2.8
5	F	338	CYS	2.8
2	B	37	HIS	2.8
5	F	13	VAL	2.8
5	F	186	LEU	2.8
5	F	226	GLU	2.8
5	F	351	VAL	2.8
1	A	56	THR	2.8
2	D	83	PHE	2.7
5	F	126	ASP	2.7
2	D	405	LEU	2.7
2	D	185	TYR	2.7
1	A	434	GLU	2.7
5	F	258	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	27	TRP	2.7
5	F	135	TYR	2.7
2	D	418	PHE	2.7
5	F	98	TYR	2.7
2	D	30	ILE	2.7
5	F	340	GLN	2.6
1	A	178	SER	2.6
2	D	276	THR	2.6
1	A	282	TYR	2.6
1	A	418	PHE	2.6
1	A	351	PHE	2.6
2	B	438	ALA	2.6
3	C	337	THR	2.6
5	F	348	GLN	2.6
1	A	255	PHE	2.5
5	F	223	THR	2.5
5	F	14	TYR	2.5
2	B	60	LYS	2.5
5	F	257	GLU	2.5
2	D	408	TYR	2.5
2	D	78	VAL	2.5
1	A	88	HIS	2.5
5	F	23	ALA	2.5
5	F	220	VAL	2.5
5	F	356	SER	2.4
1	A	316	CYS	2.4
5	F	146	VAL	2.4
3	C	437	VAL	2.4
5	F	90	SER	2.4
2	B	58	GLY	2.4
5	F	320	MET	2.4
1	A	62	VAL	2.4
2	D	334	ASN	2.4
1	A	315	CYS	2.4
4	E	44	ASP	2.4
5	F	18	SER	2.4
4	E	140	LYS	2.4
5	F	342	LEU	2.4
3	C	357	TYR	2.3
5	F	24	THR	2.3
5	F	187	GLU	2.3
5	F	353	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	97	SER	2.3
2	B	49	ILE	2.3
2	D	97	SER	2.3
5	F	314	LEU	2.3
5	F	184	LYS	2.3
5	F	204	TRP	2.3
2	D	212	ILE	2.3
5	F	346	LEU	2.3
2	D	59	ASN	2.3
1	A	163	LYS	2.3
1	A	284	GLU	2.3
4	E	138	GLU	2.3
2	B	416	MET	2.3
4	E	139	LEU	2.3
2	D	114	LEU	2.3
5	F	375	PHE	2.3
2	D	110	GLU	2.3
2	D	317	ALA	2.3
5	F	376	ILE	2.2
1	A	252	LEU	2.2
3	C	436	GLY	2.2
2	D	55	GLU	2.2
2	D	407	TRP	2.2
3	C	372	GLN	2.2
2	B	53	TYR	2.2
2	D	69	ASP	2.2
5	F	259	GLY	2.2
4	E	25	LYS	2.2
2	D	58	GLY	2.2
2	D	402	LYS	2.2
2	D	93	VAL	2.2
5	F	191	LEU	2.2
1	A	259	LEU	2.1
5	F	41	LEU	2.1
5	F	264	PHE	2.1
5	F	227	PRO	2.1
1	A	149	PHE	2.1
1	A	65	ALA	2.1
3	C	167	LEU	2.1
5	F	70	LYS	2.1
1	A	35	GLN	2.1
2	D	413	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	87	PHE	2.1
2	B	345	GLU	2.1
5	F	152	SER	2.1
2	D	168	THR	2.1
2	D	167	ASN	2.1
3	C	252	LEU	2.0
2	D	86	ILE	2.0
5	F	125	THR	2.0
2	B	62	VAL	2.0
1	A	2	ARG	2.0
1	A	67	PHE	2.0
5	F	336	PRO	2.0
2	D	92	PHE	2.0
3	C	283	HIS	2.0
2	D	70	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MG	A	506	1/1	0.62	0.50	14.85	84,84,84,84	0
11	71P	B	504	29/29	0.69	0.52	4.65	96,97,99,100	29
7	MG	A	502	1/1	0.98	0.53	2.81	68,68,68,68	0
12	CA	C	503	1/1	0.65	0.27	2.65	123,123,123,123	0
10	MES	B	503	12/12	0.95	0.32	1.46	94,95,97,99	0
7	MG	A	505	1/1	0.77	0.32	1.12	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GTP	C	501	32/32	0.96	0.30	0.78	77,79,80,81	0
7	MG	B	505	1/1	0.77	0.31	0.53	71,71,71,71	0
6	GTP	A	501	32/32	0.95	0.28	0.39	81,83,84,85	0
9	GDP	B	501	28/28	0.94	0.26	0.30	77,77,78,79	0
9	GDP	D	600	28/28	0.90	0.21	-0.24	101,102,107,109	0
7	MG	A	504	1/1	0.80	0.19	-1.02	95,95,95,95	0
7	MG	B	506	1/1	0.53	0.57	-	87,87,87,87	0
8	CL	A	503	1/1	0.95	0.09	-	98,98,98,98	0
7	MG	B	502	1/1	0.44	0.62	-	88,88,88,88	0
7	MG	C	502	1/1	0.94	0.48	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.