



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I55
Title : Crystal structure of tubulin-stathmin-TTL complex
Authors : Prota, A.E.; Bargsten, K.; Zurwerra, D.; Field, J.J.; Diaz, J.F.; Altmann, K.H.; Steinmetz, M.O.
Deposited on : 2012-11-28
Resolution : 2.20 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 (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

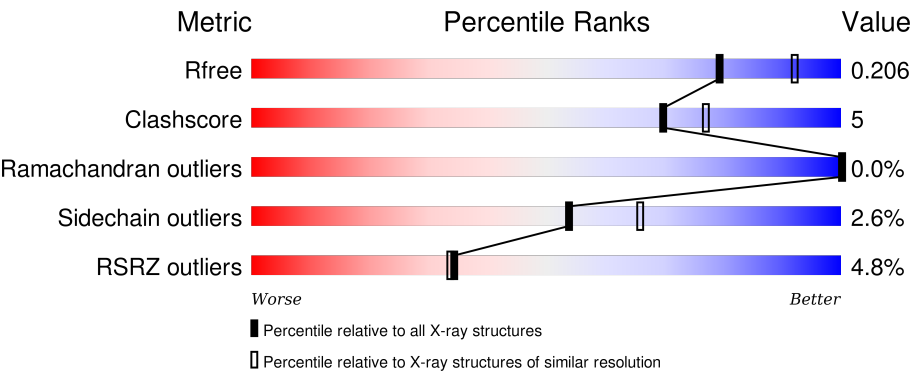
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	450	<div><div>88%9%</div><div>0%100%</div></div>
1	C	450	<div><div>88%8%</div><div>0%100%</div></div>
2	B	445	<div><div>84%11%</div><div>0%100%</div></div>
2	D	445	<div><div>3%84%10%5%</div><div>0%100%</div></div>
3	E	143	<div><div>2%78%7%13%</div><div>0%100%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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
6	MG	A	502	-	-	-	X
6	MG	C	502	-	-	-	X
6	MG	F	701	-	-	-	X
7	CA	A	505	-	-	-	X
7	CA	B	503	-	-	-	X
7	CA	C	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 36041 atoms, of which 17435 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	442	Total	C	H	N	O	S	0	7	0
			6911	2207	3421	591	668	24			
1	C	440	Total	C	H	N	O	S	0	12	0
			6899	2203	3420	586	664	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	8	0
			6685	2131	3295	579	653	27			
2	D	421	Total	C	H	N	O	S	0	5	0
			6533	2087	3213	562	644	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	124	Total	C	H	N	O	S	0	4	0
			2109	643	1067	188	205	6			

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

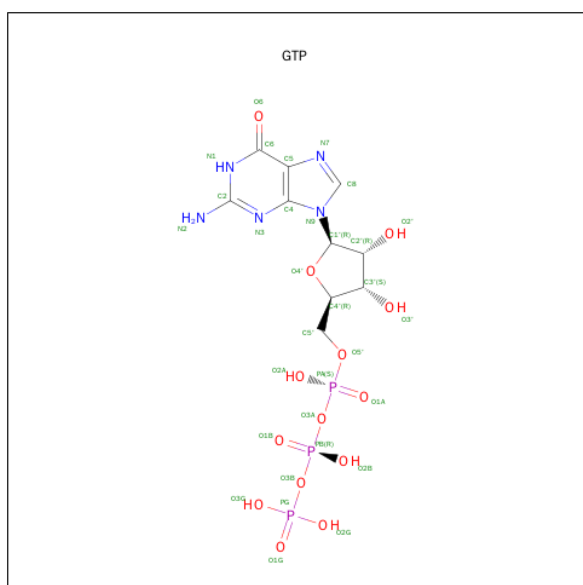
- Molecule 4 is a protein called Tubulin tyrosine ligase, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	353	Total	C	H	N	O	S	0	6	0
			5869	1885	2936	504	528	16			

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	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Mg	0	0
			2	2		

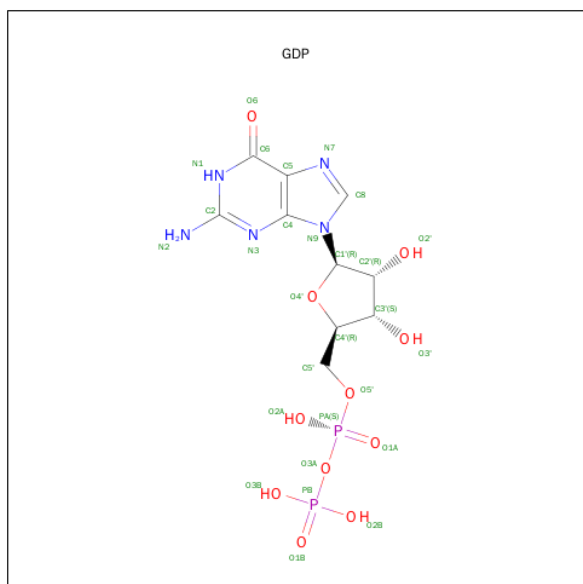
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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



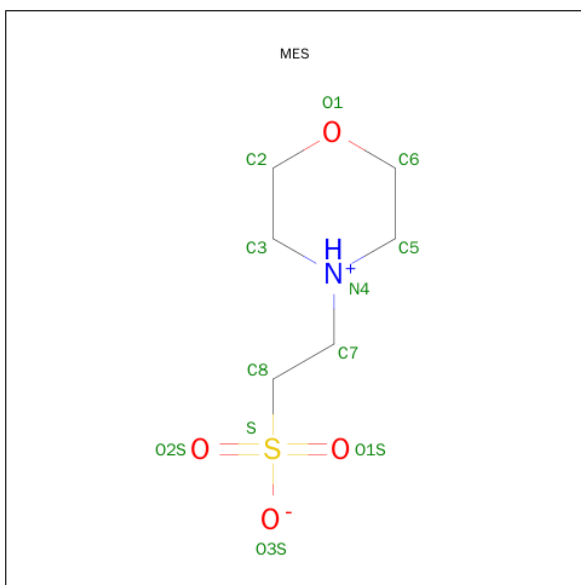
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

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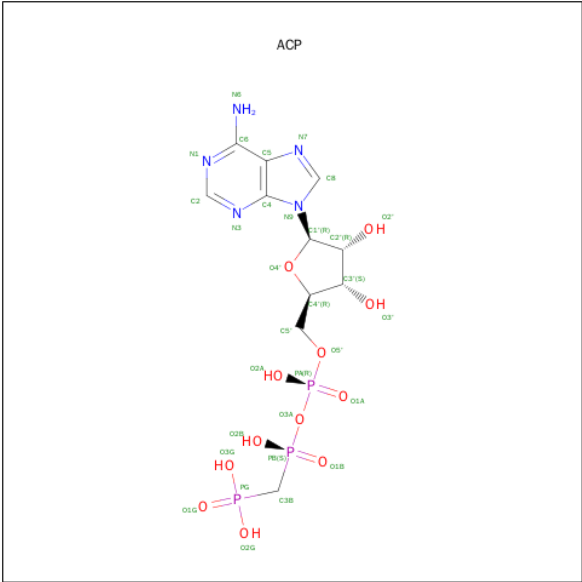
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

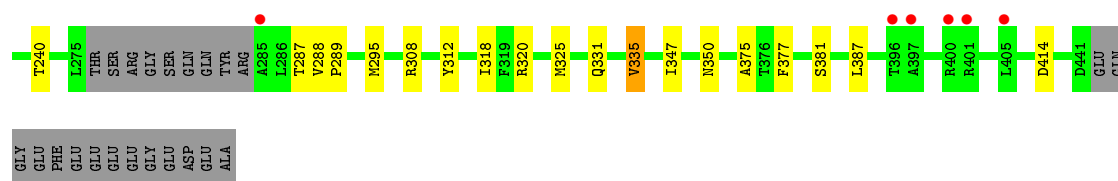
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



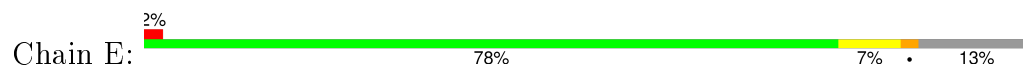
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			48	11	17	5	12	3	

- Molecule 12 is water.

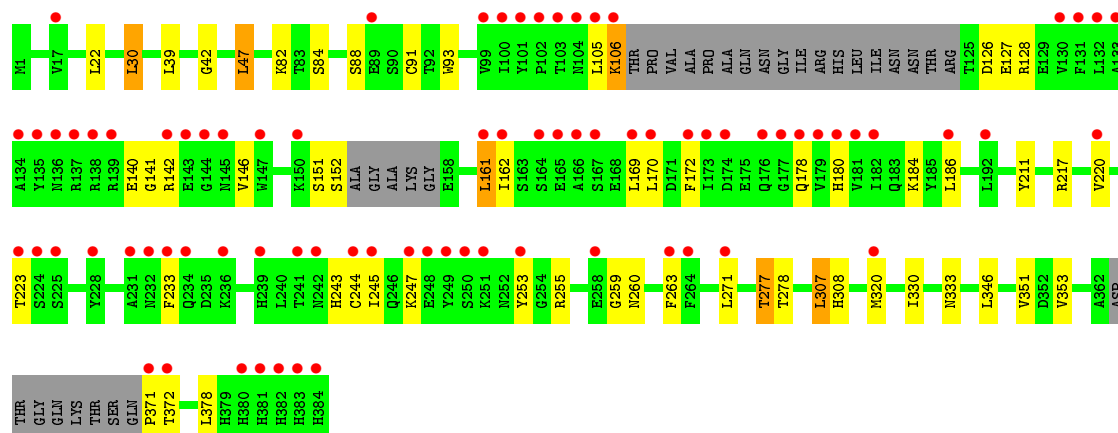
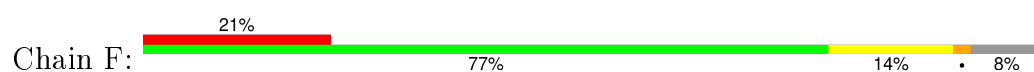
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	169	Total	O		
			169	169	0	0
12	B	157	Total	O		
			157	157	0	0
12	C	280	Total	O		
			280	280	0	0
12	D	80	Total	O		
			80	80	0	0
12	E	35	Total	O		
			35	35	0	0
12	F	44	Total	O		
			44	44	0	0



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase, TTL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.16Å 156.47Å 181.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.84 – 2.20 78.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (71.84-2.20) 99.2 (78.50-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.168 , 0.208 0.168 , 0.206	Depositor DCC
R_{free} test set	7515 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 149402 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36041	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, GTP, ACP, 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	0.41	0/3588	0.58	0/4867
1	C	0.50	0/3595	0.61	1/4881 (0.0%)
2	B	0.44	0/3495	0.55	0/4732
2	D	0.38	0/3407	0.53	0/4616
3	E	0.44	0/1063	0.50	0/1411
4	F	0.33	0/3020	0.52	0/4078
All	All	0.42	0/18168	0.56	1/24585 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ARG	NE-CZ-NH1	5.11	122.86	120.30

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	3490	3421	3408	27	0
1	C	3479	3420	3395	29	0
2	B	3390	3295	3275	32	0
2	D	3320	3213	3201	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1042	1067	1062	10	0
4	F	2933	2936	2921	37	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	2	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	0	0
10	B	24	26	25	3	0
11	F	31	17	14	6	0
12	A	169	0	0	1	0
12	B	157	0	0	2	0
12	C	280	0	0	5	0
12	D	80	0	0	0	0
12	E	35	0	0	0	0
12	F	44	0	0	1	0
All	All	18606	17435	17349	159	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 5.

All (159) 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:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.14	0.88
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.29	0.72
1:C:308:ARG:NE	12:C:802:HOH:O	2.23	0.71
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.31	0.69
2:B:199:ASP:OD2	10:B:504:MES:H32	1.94	0.68
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.34	0.67
3:E:143:ALA:HA	3:E:144:SER:C	2.15	0.67
4:F:105:LEU:O	4:F:106:LYS:HB2	1.95	0.65
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.32	0.63
2:D:175:PRO:HA	2:D:178:SER:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:THR:HG22	2:D:181:VAL:HA	1.81	0.62
1:C:361:THR:HG23	12:C:871:HOH:O	2.00	0.61
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.82	0.61
2:B:420:GLU:OE2	12:B:695:HOH:O	2.17	0.60
1:C:250:VAL:HG22	1:C:255:PHE:CE2	2.37	0.59
4:F:320[B]:MET:SD	11:F:703:ACP:C2	2.91	0.59
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.42	0.59
1:A:450:GLU:OXT	11:F:703:ACP:O3G	2.21	0.58
2:D:180:THR:HG22	2:D:181:VAL:CB	2.34	0.57
2:D:180:THR:HG22	2:D:181:VAL:CA	2.35	0.57
2:B:192:HIS:NE2	2:B:424[B]:ASN:OD1	2.38	0.56
2:B:158:ARG:CZ	10:B:504:MES:H21	2.35	0.56
2:B:124:LYS:HD3	2:B:124:LYS:O	2.06	0.56
1:C:372:GLN:NE2	12:C:809:HOH:O	2.38	0.56
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.37	0.55
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.86	0.55
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.34	0.55
3:E:143:ALA:CA	3:E:144:SER:C	2.75	0.55
4:F:320[B]:MET:HE2	4:F:330:ILE:HD11	1.88	0.54
2:B:39[A]:ASP:OD1	2:B:40:SER:N	2.41	0.54
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.91	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.08	0.53
4:F:42:GLY:HA3	4:F:47:LEU:CD2	2.39	0.53
2:D:106:GLY:O	2:D:111:GLY:HA3	2.10	0.53
1:A:193[A]:THR:HG23	12:A:663:HOH:O	2.08	0.53
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.42	0.52
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	2.98	0.51
2:B:285:ALA:HA	12:B:683:HOH:O	2.10	0.51
2:D:287:THR:HB	2:D:289:PRO:HD2	1.93	0.50
2:B:124:LYS:CD	2:B:124:LYS:C	2.80	0.50
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.46	0.50
1:C:312:TYR:CD2	1:C:315[B]:CYS:SG	3.04	0.50
4:F:106:LYS:HA	4:F:106:LYS:HE3	1.93	0.49
2:B:192:HIS:CE1	2:B:424[B]:ASN:OD1	2.66	0.49
2:D:331:GLN:O	2:D:335:VAL:HG23	2.13	0.49
2:B:275:LEU:HG	2:B:300:ASN:ND2	2.27	0.49
1:C:221:ARG:HG3	2:D:325:MET:HG3	1.94	0.49
4:F:84:SER:O	4:F:88:SER:N	2.45	0.49
11:F:703:ACP:H8	11:F:703:ACP:H5'2	1.95	0.49
2:D:124:LYS:C	2:D:124:LYS:HD3	2.34	0.49
2:B:287:THR:HB	2:B:289:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:53:LYS:HE2	3:E:53:LYS:N	2.28	0.48
2:B:253:ARG:NH1	10:B:504:MES:O2S	2.43	0.48
2:B:284:ARG:O	2:B:284:ARG:HG3	2.13	0.48
4:F:30:LEU:O	12:F:835:HOH:O	2.20	0.48
4:F:320[B]:MET:HE1	11:F:703:ACP:N1	2.29	0.48
4:F:244:CYS:SG	4:F:245:ILE:N	2.86	0.48
1:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.60	0.48
2:D:183:GLU:N	2:D:184:PRO:CD	2.77	0.48
4:F:371:PRO:CA	4:F:372:THR:HB	2.44	0.48
1:A:357:TYR:CE1	3:E:17:GLY:HA2	2.49	0.47
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.49	0.47
2:B:2:ARG:NH1	2:B:130:ASP:HB3	2.29	0.47
4:F:223:THR:OG1	4:F:260:ASN:HB3	2.15	0.47
1:C:336:LYS:HE3	1:C:351:PHE:CZ	2.49	0.47
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.96	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.96	0.47
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.07	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.47
4:F:141:GLY:O	4:F:142:ARG:HB2	2.15	0.47
3:E:143:ALA:N	3:E:144:SER:HB3	2.30	0.46
2:B:288:VAL:N	2:B:289:PRO:CD	2.78	0.46
4:F:320[B]:MET:SD	11:F:703:ACP:N3	2.88	0.46
1:A:209:ILE:HD11	1:A:302:MET:SD	2.55	0.46
1:C:270:ALA:CB	1:C:302[B]:MET:SD	3.03	0.46
1:A:263:PRO:O	1:A:266:HIS:HD2	1.99	0.46
4:F:106:LYS:HA	4:F:106:LYS:CE	2.46	0.46
2:D:180:THR:CG2	2:D:181:VAL:HA	2.46	0.46
4:F:141:GLY:O	4:F:142:ARG:CB	2.64	0.46
1:C:318:LEU:N	1:C:318:LEU:HD23	2.30	0.46
4:F:126:ASP:OD2	4:F:127:GLU:N	2.49	0.46
3:E:6:MET:SD	3:E:24:LEU:CD2	3.04	0.45
4:F:220[A]:VAL:HG12	4:F:263:PHE:CD1	2.51	0.45
2:B:106:GLY:O	2:B:111:GLY:HA3	2.17	0.45
4:F:161:LEU:HD21	4:F:169:LEU:HA	1.99	0.45
2:B:295:MET:HE3	2:B:375:ALA:HB1	1.98	0.45
1:A:386:GLU:O	1:A:390[A]:ARG:HD3	2.16	0.45
2:B:2:ARG:CZ	2:B:2:ARG:HB2	2.46	0.45
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.52	0.45
2:D:318:ILE:HD12	2:D:318:ILE:N	2.33	0.44
2:D:180:THR:HG22	2:D:181:VAL:HB	1.98	0.44
4:F:243:HIS:O	4:F:243:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.48	0.44
4:F:371:PRO:HA	4:F:372:THR:C	2.37	0.44
4:F:371:PRO:HA	4:F:372:THR:HB	1.98	0.44
1:A:97:GLU:HB2	2:B:1:MET:HG2	1.99	0.44
2:D:387:LEU:C	2:D:387:LEU:HD23	2.38	0.44
1:A:60:LYS:CE	1:A:85:GLN:O	2.65	0.44
1:C:234:ILE:CD1	1:C:302[A]:MET:SD	3.05	0.44
2:D:171:VAL:HA	2:D:204:ILE:O	2.18	0.44
4:F:247:LYS:HA	4:F:253:TYR:CD2	2.53	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.18	0.43
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.00	0.43
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.53	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.43
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.43
2:D:312:TYR:CD2	2:D:381:SER:HB2	2.54	0.43
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.53	0.43
2:D:295:MET:CE	2:D:375:ALA:HB1	2.49	0.43
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.00	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.19	0.43
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.01	0.43
4:F:146:VAL:HG21	4:F:233:PHE:CE2	2.54	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.01	0.43
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.54	0.43
4:F:140:GLU:HG2	4:F:141:GLY:N	2.33	0.43
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.49	0.43
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.54	0.43
1:C:104:ALA:HB2	1:C:413:MET:SD	2.59	0.42
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.42
4:F:333:ASN:ND2	11:F:703:ACP:O2G	2.51	0.42
4:F:128:ARG:HG3	4:F:170:LEU:CD2	2.48	0.42
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.13	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.42
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.85	0.42
2:B:332:MET:O	2:B:335:VAL:HG22	2.20	0.42
1:C:250:VAL:HG22	1:C:255:PHE:CZ	2.54	0.41
1:A:413:MET:CE	1:A:418:PHE:CE1	3.03	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.41
1:A:141:PHE:CE2	1:A:170:SER:HB3	2.56	0.41
2:D:31:ASP:C	2:D:31:ASP:OD1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:259:GLY:HA2	4:F:260:ASN:HA	1.83	0.41
4:F:161:LEU:HD23	4:F:172:PHE:HB3	2.03	0.41
1:A:77:GLU:HA	1:A:80:THR:HG22	2.02	0.41
2:B:226:ASP:OD1	2:B:278:ARG:NH1	2.53	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.02	0.41
1:C:1:MET:O	12:C:792:HOH:O	2.22	0.41
1:A:136:LEU:CD2	1:A:167:LEU:HB2	2.50	0.41
4:F:186:LEU:HG	4:F:320[B]:MET:HE3	2.03	0.41
2:B:1:MET:SD	2:B:133:GLN:HB3	2.61	0.41
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.38	0.41
2:D:288:VAL:N	2:D:289:PRO:CD	2.83	0.41
2:B:177:VAL:HG21	2:B:210:TYR:HB2	2.03	0.41
1:C:209:ILE:HD11	1:C:302[A]:MET:SD	2.61	0.40
2:B:2:ARG:HB3	2:B:2:ARG:NH1	2.36	0.40
4:F:277:THR:HG22	4:F:278:THR:H	1.85	0.40
2:B:7:ILE:O	2:B:137:LEU:HA	2.21	0.40
2:D:83:PHE:O	2:D:86:ILE:HG22	2.21	0.40
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.14	0.40
1:C:128:GLN:OE1	12:C:791:HOH:O	2.22	0.40
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.40
4:F:161:LEU:HD12	4:F:162:ILE:N	2.36	0.40
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.04	0.40
2:B:216:THR:HG22	2:B:217:LEU:HD23	2.03	0.40
3:E:137:LYS:HA	3:E:140:LYS:HD2	2.04	0.40
4:F:186:LEU:HD23	4:F:320[B]:MET:HE1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/450 (99%)	439 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	449/450 (100%)	438 (98%)	11 (2%)	0	100	100
2	B	429/445 (96%)	418 (97%)	11 (3%)	0	100	100
2	D	421/445 (95%)	408 (97%)	12 (3%)	1 (0%)	52	59
3	E	124/143 (87%)	121 (98%)	3 (2%)	0	100	100
4	F	351/384 (91%)	332 (95%)	19 (5%)	0	100	100
All	All	2219/2317 (96%)	2156 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	81	GLY

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	380/378 (100%)	377 (99%)	3 (1%)	86	93
1	C	382/378 (101%)	375 (98%)	7 (2%)	66	79
2	B	376/383 (98%)	370 (98%)	6 (2%)	70	82
2	D	367/383 (96%)	358 (98%)	9 (2%)	55	67
3	E	115/127 (91%)	109 (95%)	6 (5%)	29	33
4	F	325/342 (95%)	304 (94%)	21 (6%)	21	23
All	All	1945/1991 (98%)	1893 (97%)	52 (3%)	54	64

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	166	LYS
1	A	450	GLU
2	B	139	HIS
2	B	190	SER

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Mol	Chain	Res	Type
2	B	200	GLU
2	B	220	THR
2	B	277	SER
2	B	282	GLN
1	C	71	GLU
1	C	218	ASP
1	C	284	GLU
1	C	302[A]	MET
1	C	302[B]	MET
1	C	318	LEU
1	C	381	THR
2	D	15	GLN
2	D	39	ASP
2	D	50	ASN
2	D	75	MET
2	D	139	HIS
2	D	180	THR
2	D	308	ARG
2	D	335	VAL
2	D	414	ASP
3	E	6	MET
3	E	53	LYS
3	E	96	MET
3	E	103	GLN
3	E	135	LYS
3	E	140	LYS
4	F	22	LEU
4	F	30	LEU
4	F	39	LEU
4	F	47	LEU
4	F	106	LYS
4	F	152	SER
4	F	161	LEU
4	F	178	GLN
4	F	184	LYS
4	F	211	TYR
4	F	217	ARG
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	277	THR

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Mol	Chain	Res	Type
4	F	307	LEU
4	F	346	LEU
4	F	351	VAL
4	F	353	VAL
4	F	378	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	283	HIS
1	A	301	GLN
1	C	197	HIS
4	F	379	HIS

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 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	25,34,34	1.02	1 (4%)	32,54,54	1.20	5 (15%)
9	GDP	B	501	6	23,30,30	1.60	6 (26%)	28,47,47	1.89	3 (10%)
10	MES	B	504	-	12,12,12	1.90	1 (8%)	16,16,16	1.50	2 (12%)
10	MES	B	505	-	12,12,12	2.01	1 (8%)	16,16,16	1.46	2 (12%)
5	GTP	C	501	6	25,34,34	0.95	1 (4%)	32,54,54	1.08	4 (12%)
9	GDP	D	600	6	23,30,30	1.32	3 (13%)	28,47,47	1.55	4 (14%)
11	ACP	F	703	6	25,33,33	1.65	6 (24%)	31,52,52	2.75	7 (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
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	1/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	600	6	-	0/12/32/32	0/3/3/3
11	ACP	F	703	6	-	0/15/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-5.98	1.67	1.78
10	B	504	MES	C8-S	-5.77	1.67	1.78
11	F	703	ACP	C2'-C3'	-3.05	1.45	1.53
9	B	501	GDP	C6-N1	-2.89	1.32	1.36
11	F	703	ACP	O3'-C3'	-2.28	1.37	1.43
11	F	703	ACP	O5'-C5'	-2.18	1.35	1.44
11	F	703	ACP	PG-O2G	2.14	1.60	1.54
9	D	600	GDP	C2-N2	2.19	1.35	1.32
9	B	501	GDP	O4'-C1'	2.33	1.44	1.41
9	B	501	GDP	C2-N3	2.44	1.36	1.33
9	B	501	GDP	C5-C4	2.61	1.46	1.40
11	F	703	ACP	PG-O3G	2.62	1.61	1.54
9	D	600	GDP	C5-C4	2.89	1.47	1.40
9	B	501	GDP	C2-N2	3.21	1.37	1.32
5	C	501	GTP	C2-N3	3.29	1.37	1.33
9	D	600	GDP	C6-C5	3.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C6-C5	3.79	1.48	1.41
5	A	501	GTP	C2-N3	3.89	1.38	1.33
11	F	703	ACP	C6-N6	4.21	1.47	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	703	ACP	N3-C2-N1	-8.77	122.18	128.89
11	F	703	ACP	O4'-C1'-N9	-6.70	94.06	108.10
9	B	501	GDP	C1'-N9-C4	-3.96	120.96	126.94
11	F	703	ACP	PA-O3A-PB	-3.92	121.72	132.73
5	C	501	GTP	C4-C5-N7	-3.19	106.55	109.48
9	D	600	GDP	C4-C5-N7	-3.00	106.72	109.48
9	B	501	GDP	C4-C5-N7	-2.81	106.89	109.48
5	A	501	GTP	C1'-N9-C4	-2.79	122.73	126.94
5	A	501	GTP	PA-O3A-PB	-2.53	125.63	132.73
9	D	600	GDP	PA-O3A-PB	-2.48	124.37	132.67
5	A	501	GTP	C4-C5-N7	-2.35	107.32	109.48
9	D	600	GDP	C1'-N9-C4	-2.24	123.57	126.94
5	C	501	GTP	PB-O3B-PG	-2.21	125.26	132.67
11	F	703	ACP	C5'-C4'-C3'	-2.05	107.09	115.21
5	A	501	GTP	PB-O3B-PG	-2.04	125.82	132.67
5	C	501	GTP	PA-O3A-PB	-2.02	127.06	132.73
5	A	501	GTP	O3A-PA-O5'	-2.02	97.58	102.94
10	B	505	MES	C7-C8-S	-2.00	108.73	112.99
11	F	703	ACP	O3A-PA-O5'	2.01	108.27	102.94
5	C	501	GTP	O2B-PB-O3A	2.14	114.79	105.09
10	B	504	MES	O1S-S-C8	2.31	111.89	106.41
10	B	505	MES	C5-N4-C3	2.70	115.43	109.76
11	F	703	ACP	O5'-C5'-C4'	2.97	120.08	109.12
10	B	504	MES	C5-N4-C3	4.03	118.23	109.76
9	D	600	GDP	C6-N1-C2	4.93	122.98	120.20
9	B	501	GDP	C6-N1-C2	6.96	124.13	120.20
11	F	703	ACP	C2'-C1'-N9	7.52	125.78	114.29

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	505	MES	C2-C3-C5-C6-N4-O1

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	3	0
11	F	703	ACP	6	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, 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	442/450 (98%)	0.03	5 (1%)	82 82	29, 46, 79, 143	0
1	C	440/450 (97%)	0.27	3 (0%)	89 88	23, 35, 66, 116	1 (0%)
2	B	425/445 (95%)	0.16	3 (0%)	89 88	23, 43, 79, 128	2 (0%)
2	D	421/445 (94%)	0.21	13 (3%)	52 51	29, 56, 91, 150	7 (1%)
3	E	124/143 (86%)	0.25	3 (2%)	62 61	32, 62, 107, 141	0
4	F	353/384 (91%)	1.07	79 (22%)	1 1	39, 72, 148, 175	0
All	All	2205/2317 (95%)	0.32	106 (4%)	34 34	23, 49, 104, 175	10 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	9.4
4	F	173	ILE	8.4
1	A	440	VAL	8.0
4	F	130	VAL	6.6
4	F	134	ALA	6.5
4	F	100	ILE	6.5
4	F	182	ILE	6.5
4	F	169	LEU	6.1
4	F	381	HIS	6.0
4	F	249	TYR	5.8
4	F	106	LYS	5.6
4	F	103	THR	5.5
2	D	285	ALA	5.5
4	F	133	ALA	5.1
4	F	101	TYR	5.0
4	F	178	GLN	4.9
4	F	186	LEU	4.8
4	F	104	ASN	4.6
4	F	170	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	439	SER	4.5
4	F	179	VAL	4.5
2	D	57	THR	4.5
2	D	400	ARG	4.4
4	F	320[A]	MET	4.1
4	F	233	PHE	4.1
2	D	177	VAL	4.1
4	F	225	SER	4.1
4	F	251	LYS	4.0
4	F	271[A]	LEU	4.0
4	F	382	HIS	4.0
4	F	176	GLN	4.0
2	D	405	LEU	3.9
4	F	138	ARG	3.9
2	B	284	ARG	3.9
4	F	99	VAL	3.8
4	F	181	VAL	3.7
4	F	253	TYR	3.7
4	F	161	LEU	3.6
4	F	137	ARG	3.6
4	F	139	ARG	3.6
4	F	142	ARG	3.6
4	F	372	THR	3.6
1	C	211[A]	ASP	3.5
2	B	438	ALA	3.4
4	F	383	HIS	3.4
4	F	384	HIS	3.4
4	F	380	HIS	3.3
4	F	172	PHE	3.2
2	D	401	ARG	3.2
4	F	131	PHE	3.1
1	A	450	GLU	3.1
4	F	177	GLY	3.1
4	F	132	LEU	3.0
2	D	212	ILE	3.0
2	D	182	VAL	3.0
1	C	340	SER	3.0
2	D	397	ALA	2.9
4	F	162	ILE	2.9
2	D	217	LEU	2.9
4	F	174	ASP	2.9
4	F	180	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	218	LYS	2.9
4	F	245	ILE	2.8
4	F	167	SER	2.7
4	F	144	GLY	2.7
4	F	102	PRO	2.7
2	D	82	PRO	2.6
1	A	262	TYR	2.5
4	F	136	ASN	2.5
4	F	231	ALA	2.5
4	F	220[A]	VAL	2.5
4	F	244	CYS	2.5
4	F	241	THR	2.5
4	F	143	GLU	2.5
4	F	224	SER	2.5
4	F	145	ASN	2.5
4	F	223	THR	2.4
4	F	150	LYS	2.4
4	F	192	LEU	2.4
4	F	147	TRP	2.4
4	F	234	GLN	2.4
2	D	396	THR	2.3
4	F	166	ALA	2.3
4	F	250	SER	2.3
4	F	247	LYS	2.3
3	E	12[A]	ASN	2.2
4	F	165	GLU	2.2
4	F	232	ASN	2.2
4	F	264	PHE	2.2
1	C	285	GLN	2.2
2	B	278	ARG	2.2
4	F	258	GLU	2.2
4	F	236	LYS	2.1
4	F	371	PRO	2.1
4	F	239	HIS	2.1
4	F	263	PHE	2.1
4	F	248	GLU	2.1
4	F	164	SER	2.1
1	A	438	ASP	2.1
3	E	28	SER	2.1
4	F	242	ASN	2.0
4	F	135	TYR	2.0
3	E	25	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	89	GLU	2.0
4	F	17	VAL	2.0
4	F	228	TYR	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
6	MG	A	502	1/1	0.93	0.24	8.24	38,38,38,38	0
6	MG	C	502	1/1	0.95	0.22	7.52	33,33,33,33	0
7	CA	A	505	1/1	0.90	0.24	4.87	95,95,95,95	0
7	CA	B	503	1/1	0.94	0.26	4.84	91,91,91,91	0
7	CA	C	503	1/1	0.96	0.23	4.79	55,55,55,55	0
6	MG	F	701	1/1	0.93	0.37	3.78	93,93,93,93	0
9	GDP	B	501	28/28	0.99	0.19	1.58	19,30,41,42	0
5	GTP	A	501	32/32	0.99	0.16	1.29	24,33,40,45	0
5	GTP	C	501	32/32	0.99	0.16	1.15	22,27,34,37	0
7	CA	A	503	1/1	0.96	0.14	0.86	60,60,60,60	0
10	MES	B	505	12/12	0.97	0.14	0.33	71,86,102,102	0
10	MES	B	504	12/12	0.98	0.14	0.03	48,64,83,93	0
9	GDP	D	600	28/28	0.97	0.13	-0.47	41,54,75,77	0
11	ACP	F	703	31/31	0.91	0.16	-1.06	58,94,138,143	0
6	MG	B	506	1/1	0.89	0.32	-	60,60,60,60	0
6	MG	F	702	1/1	0.97	0.16	-	94,94,94,94	0
8	CL	A	504	1/1	0.91	0.15	-	67,67,67,67	0
6	MG	D	601	1/1	0.82	0.16	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	B	502	1/1	0.98	0.28	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.