Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:32 PM GMT

PDB ID	:	4F61
Title	:	Tubulin:Stathmin-like domain complex
Authors	:	Gigant, B.; Mignot, I.; Knossow, M.
Deposited on	:	2012-05-14
Resolution	:	4.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

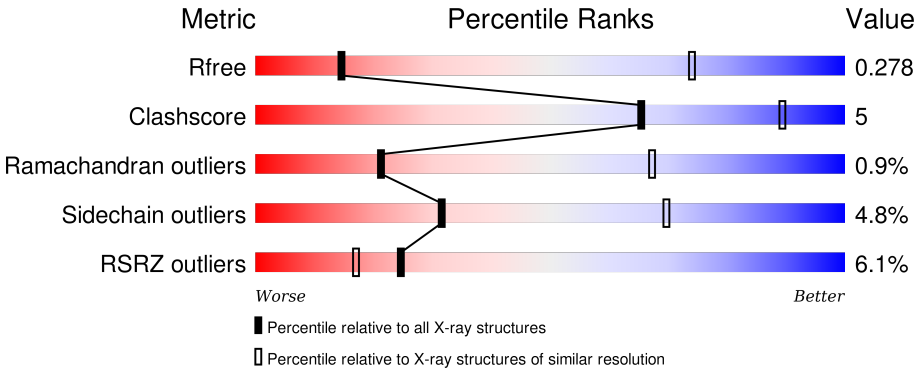
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.17 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	1030 (4.76-3.60)
Clashscore	102246	1130 (4.76-3.60)
Ramachandran outliers	100387	1076 (4.76-3.60)
Sidechain outliers	100360	1061 (4.76-3.60)
RSRZ outliers	91569	1034 (4.76-3.60)

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	5% 82% 13% •
1	C	451	9% 81% 14% • •
1	E	451	8% 84% 11% • •
1	G	451	5% 82% 13% • •
2	B	445	5% 83% 13% • •

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Mol	Chain	Length	Quality of chain
2	D	445	9% 82% 14%
2	F	445	6% 82% 15%
2	H	445	2% 80% 16%
3	I	240	4% 63% 30%

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	GDP	F	600	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29129 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3380	2141	574	643	22			
1	C	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			
1	E	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			
1	G	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
E	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
E	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
G	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
G	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3383	2124	576	657	26			
2	D	432	Total	C	N	O	S	0	0	0
			3383	2124	576	657	26			
2	F	432	Total	C	N	O	S	0	0	0
			3383	2124	576	657	26			
2	H	431	Total	C	N	O	S	0	0	0
			3375	2116	579	655	25			

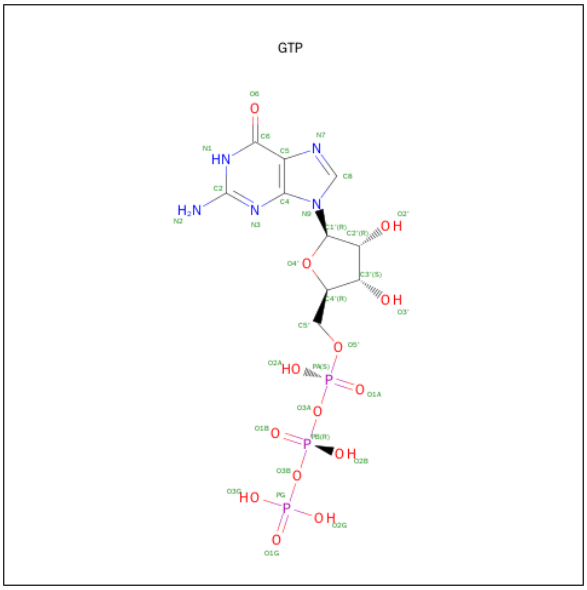
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
F	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
H	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9

- Molecule 3 is a protein called Stathmin-like domain R4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	234	Total	C	N	O	S	0	0	0
			1925	1185	362	369	9			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

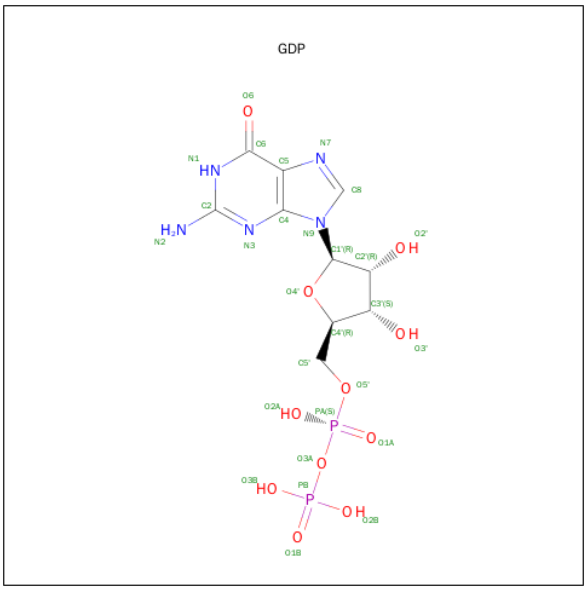


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

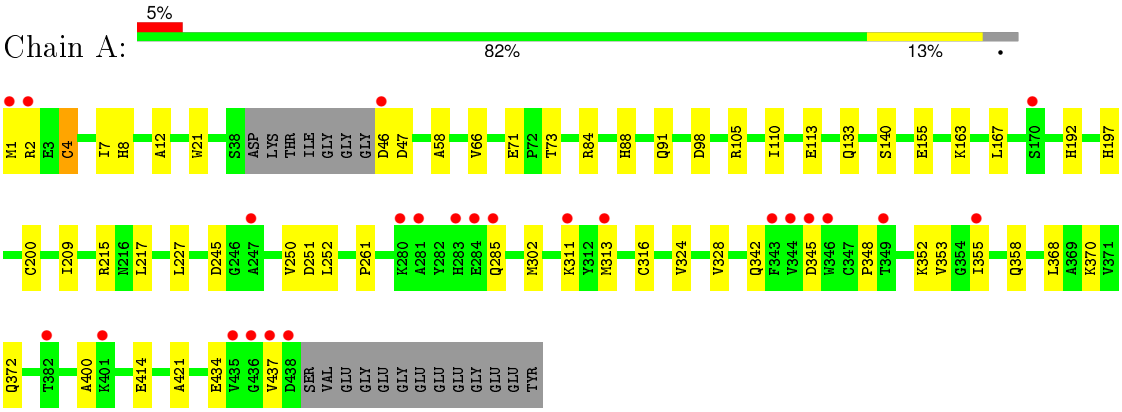


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P 28 10 5 11 2	0	0
6	D	1	Total C N O P 28 10 5 11 2	0	0
6	F	1	Total C N O P 28 10 5 11 2	0	0
6	H	1	Total C N O P 28 10 5 11 2	0	0

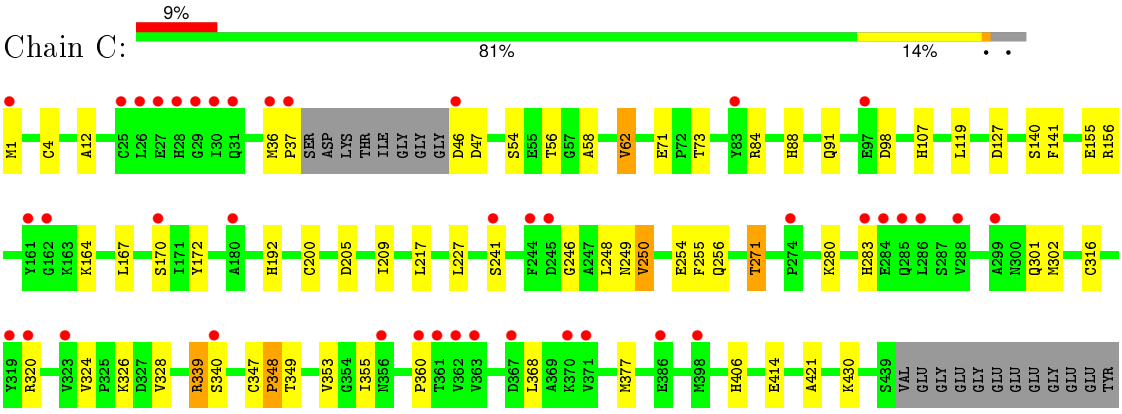
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

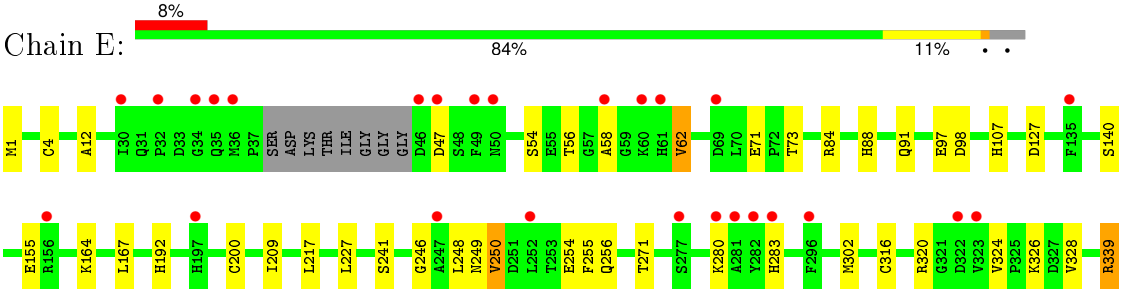
- Molecule 1: Tubulin alpha chain

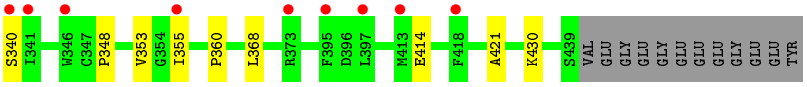


- Molecule 1: Tubulin alpha chain



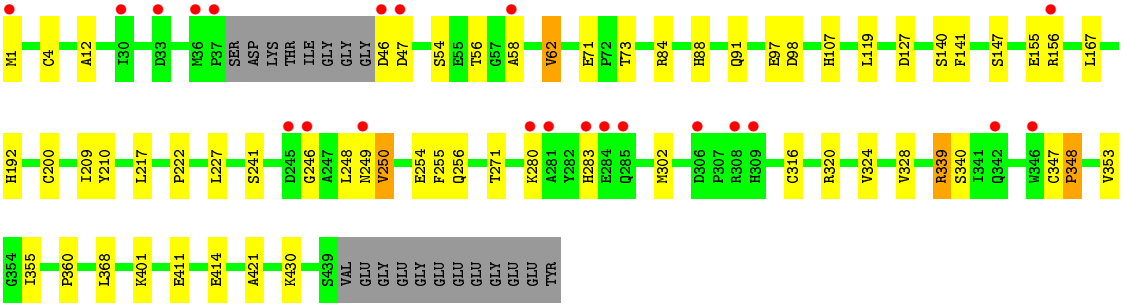
- Molecule 1: Tubulin alpha chain





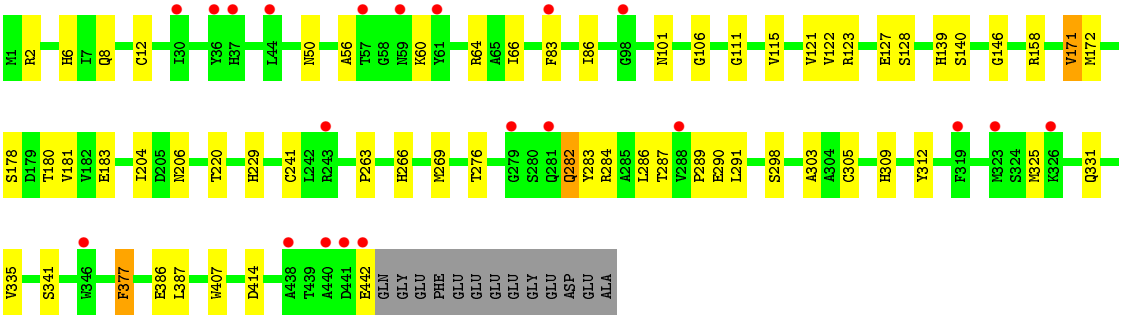
• Molecule 1: Tubulin alpha chain

Chain G:



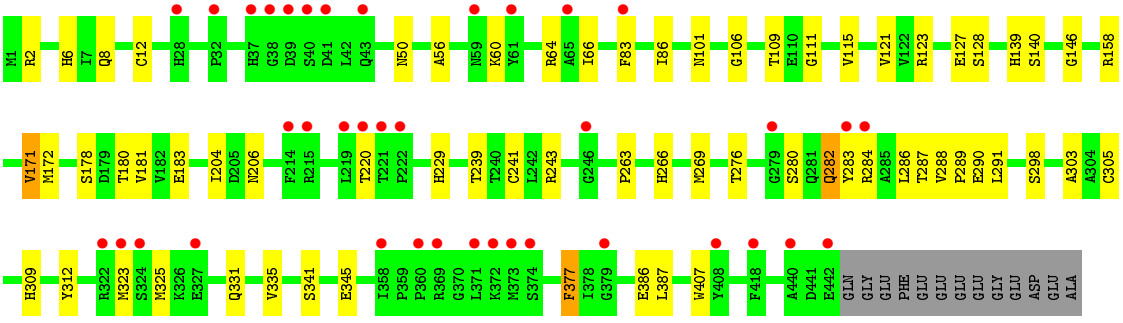
• Molecule 2: Tubulin beta chain

Chain B:



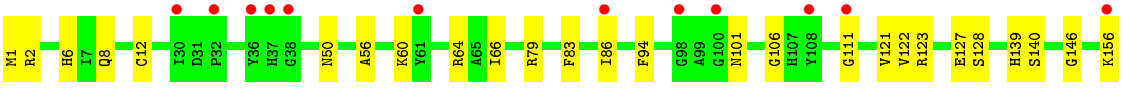
• Molecule 2: Tubulin beta chain

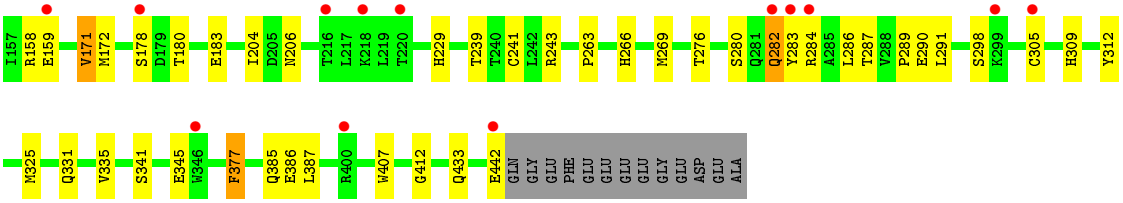
Chain D:



• Molecule 2: Tubulin beta chain

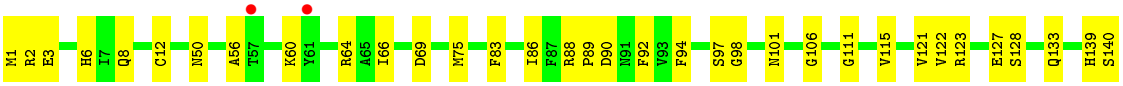
Chain F:

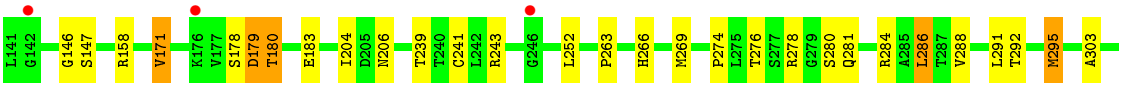


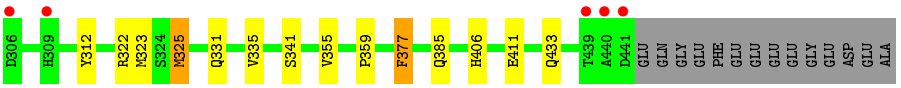


• Molecule 2: Tubulin beta chain

Chain H:

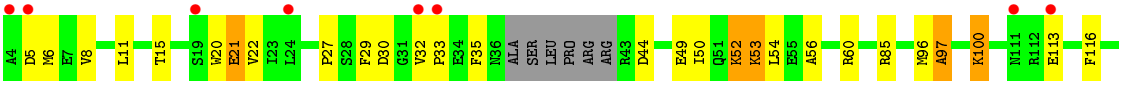


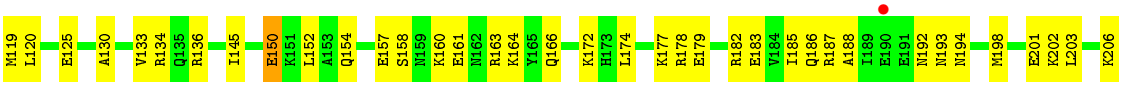


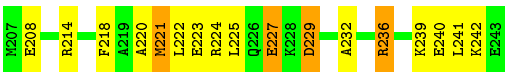


• Molecule 3: Stathmin-like domain R4

Chain I:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	639.74Å 66.10Å 128.13Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	49.04 – 4.17 49.04 – 4.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.04-4.17) 98.7 (49.04-4.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.241 , 0.261 0.255 , 0.278	Depositor DCC
R_{free} test set	2009 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	150.8	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 182.8	EDS
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	2 of 40334 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	29129	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, GTP, MG

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	0.51	0/3457	0.72	0/4693
1	C	0.45	0/3427	0.70	0/4655
1	E	0.47	0/3427	0.70	0/4655
1	G	0.52	0/3427	0.73	0/4655
2	B	0.48	0/3458	0.70	0/4686
2	D	0.44	0/3458	0.69	0/4686
2	F	0.47	0/3458	0.70	0/4686
2	H	0.63	0/3449	0.81	4/4673 (0.1%)
3	I	0.59	0/1947	0.91	0/2592
All	All	0.50	0/29508	0.73	4/39981 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	179	ASP	C-N-CA	-6.06	106.56	121.70
2	H	281	GLN	C-N-CA	5.82	136.25	121.70
2	H	180	THR	N-CA-CB	5.78	121.28	110.30
2	H	97	SER	N-CA-C	5.58	126.06	111.00

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	3380	0	3290	25	1
1	C	3352	0	3253	32	0
1	E	3352	0	3253	24	0
1	G	3352	0	3253	27	0
2	B	3383	0	3246	38	0
2	D	3383	0	3246	38	0
2	F	3383	0	3246	38	0
2	H	3375	0	3246	49	1
3	I	1925	0	1912	40	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	E	32	0	12	0	0
4	G	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	1	0
6	F	28	0	12	1	0
6	H	28	0	12	1	0
All	All	29129	0	28041	287	1

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 (287) 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:H:1:MET:SD	2:H:1:MET:CE	2.01	1.48
1:G:250:VAL:HG23	1:G:254:GLU:HB3	1.36	1.07
1:E:250:VAL:HG23	1:E:254:GLU:HB3	1.40	1.03
1:C:250:VAL:HG23	1:C:254:GLU:HB3	1.39	1.01
2:H:286:LEU:HD12	2:H:291:LEU:HD23	1.44	0.97
2:H:295:MET:SD	2:H:377:PHE:HB2	2.09	0.92
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.66	0.78
2:H:292:THR:HG22	2:H:335:VAL:HG21	1.62	0.78
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.67	0.76
1:G:71:GLU:HB3	1:G:98:ASP:HB3	1.67	0.75
2:H:206:ASN:HD21	6:H:600:GDP:HN22	1.34	0.75
1:E:250:VAL:HG22	1:E:255:PHE:CD1	2.22	0.74
2:F:206:ASN:HD21	6:F:600:GDP:HN22	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:GLU:HB3	1:E:98:ASP:HB3	1.70	0.73
2:B:206:ASN:HD21	6:B:600:GDP:HN22	1.33	0.72
1:C:250:VAL:HG22	1:C:255:PHE:CD1	2.24	0.72
1:G:250:VAL:HG22	1:G:255:PHE:CD1	2.25	0.71
2:D:206:ASN:HD21	6:D:600:GDP:HN22	1.40	0.69
1:A:245:ASP:HB3	3:I:15:THR:HB	1.77	0.66
2:D:263:PRO:O	2:D:266:HIS:HD2	1.80	0.65
3:I:198:MET:SD	3:I:202:LYS:HD2	2.36	0.65
3:I:11:LEU:HG	3:I:20:TRP:HA	1.79	0.65
1:E:328:VAL:HG11	1:E:353:VAL:HG11	1.80	0.64
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.32	0.64
3:I:192:ASN:C	3:I:194:ASN:H	2.01	0.64
2:H:133:GLN:HE22	2:H:252:LEU:H	1.43	0.64
2:B:263:PRO:O	2:B:266:HIS:HD2	1.81	0.63
2:F:263:PRO:O	2:F:266:HIS:HD2	1.81	0.63
2:H:263:PRO:O	2:H:266:HIS:HD2	1.82	0.63
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.80	0.62
2:H:92:PHE:HD2	2:H:94:PHE:HE2	1.47	0.62
2:D:50:ASN:O	2:D:64:ARG:NH2	2.34	0.60
1:G:328:VAL:HG11	1:G:353:VAL:HG11	1.82	0.60
2:H:322:ARG:HH22	2:H:359:PRO:HD3	1.67	0.60
2:D:229:HIS:HE1	2:D:276:THR:HG23	1.66	0.60
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.67	0.59
2:H:6:HIS:HE1	2:H:8:GLN:HG3	1.67	0.59
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.83	0.59
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.68	0.58
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.68	0.58
2:F:309:HIS:HD2	2:F:386:GLU:OE1	1.86	0.58
2:F:172:MET:HG3	2:F:387:LEU:HD11	1.86	0.58
2:F:180:THR:HG23	2:F:183:GLU:HG3	1.86	0.57
1:G:248:LEU:HB2	1:G:355:ILE:H	1.69	0.57
2:F:6:HIS:HE1	2:F:8:GLN:HG3	1.70	0.57
2:B:229:HIS:HE1	2:B:276:THR:HG23	1.70	0.57
2:F:229:HIS:HE1	2:F:276:THR:HG23	1.69	0.57
1:G:88:HIS:HB2	1:G:91:GLN:HE21	1.70	0.56
2:B:180:THR:HG23	2:B:183:GLU:HG3	1.87	0.56
1:C:56:THR:HG23	1:C:58:ALA:H	1.71	0.56
2:F:159:GLU:HA	3:I:174:LEU:HD13	1.88	0.56
2:D:180:THR:HG23	2:D:183:GLU:HG3	1.87	0.56
3:I:52:LYS:O	3:I:56:ALA:HB2	2.04	0.56
1:G:56:THR:HG23	1:G:58:ALA:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:VAL:HG22	3:I:22:VAL:HG22	1.86	0.56
2:H:56:ALA:HB3	2:H:60:LYS:HG3	1.87	0.56
2:F:56:ALA:HB3	2:F:60:LYS:HG3	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.55
1:E:88:HIS:HB2	1:E:91:GLN:HE21	1.71	0.55
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.89	0.55
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.55	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.55
1:A:105:ARG:HB3	1:A:110:ILE:CD1	2.37	0.55
2:B:286:LEU:HD12	2:B:291:LEU:HD23	1.89	0.55
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.53	0.55
3:I:52:LYS:HE2	3:I:53:LYS:HG3	1.89	0.55
3:I:232:ALA:O	3:I:236:ARG:HD3	2.07	0.54
1:E:56:THR:HG23	1:E:58:ALA:H	1.72	0.54
2:H:286:LEU:HD12	2:H:291:LEU:CD2	2.29	0.54
2:H:75:MET:CB	2:H:94:PHE:CE2	2.90	0.54
2:B:282:GLN:CB	2:B:283:TYR:HA	2.37	0.54
2:H:295:MET:HG3	2:H:377:PHE:CD1	2.42	0.54
2:D:309:HIS:HD2	2:D:386:GLU:OE1	1.90	0.54
2:F:6:HIS:HE1	2:F:8:GLN:HE21	1.55	0.54
2:F:287:THR:HG23	2:F:289:PRO:HD2	1.89	0.54
1:A:348:PRO:HB3	3:I:27:PRO:HD3	1.89	0.54
2:H:50:ASN:O	2:H:64:ARG:NH2	2.37	0.53
2:D:286:LEU:HD12	2:D:291:LEU:HD23	1.90	0.53
2:F:286:LEU:HD12	2:F:291:LEU:HD23	1.90	0.53
2:B:50:ASN:O	2:B:64:ARG:NH2	2.36	0.53
1:E:248:LEU:HB2	1:E:355:ILE:H	1.71	0.53
2:H:6:HIS:HE1	2:H:8:GLN:HE21	1.55	0.53
1:C:54:SER:OG	1:C:62:VAL:HG13	2.08	0.52
1:G:246:GLY:H	1:G:249:ASN:HD21	1.58	0.52
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.91	0.52
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.09	0.52
2:H:6:HIS:CE1	2:H:8:GLN:HG3	2.44	0.52
2:D:139:HIS:HD2	2:D:146:GLY:O	1.93	0.52
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.43	0.52
1:G:97:GLU:HG3	2:H:1:MET:HG2	1.92	0.52
2:D:56:ALA:HB3	2:D:60:LYS:HG3	1.91	0.52
2:F:269:MET:CE	2:F:305:CYS:HB2	2.39	0.52
2:D:109:THR:HG23	3:I:134:ARG:NH2	2.25	0.52
1:G:54:SER:OG	1:G:62:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLY:H	1:C:249:ASN:HD21	1.57	0.52
1:C:248:LEU:HB2	1:C:355:ILE:H	1.74	0.52
2:B:269:MET:CE	2:B:305:CYS:HB2	2.40	0.52
2:H:180:THR:HG23	2:H:183:GLU:HG3	1.92	0.51
2:H:274:PRO:HB3	2:H:286:LEU:HG	1.92	0.51
1:A:105:ARG:HB3	1:A:110:ILE:HD12	1.93	0.51
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.93	0.51
2:F:139:HIS:HD2	2:F:146:GLY:O	1.94	0.51
3:I:160:LYS:HE2	3:I:164:LYS:HD2	1.90	0.51
3:I:185:ILE:O	3:I:188:ALA:HB3	2.10	0.51
1:E:54:SER:OG	1:E:62:VAL:HG13	2.10	0.51
2:D:282:GLN:CB	2:D:283:TYR:HA	2.40	0.51
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.92	0.51
2:B:139:HIS:HD2	2:B:146:GLY:O	1.93	0.51
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.45	0.51
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.75	0.51
2:D:269:MET:CE	2:D:305:CYS:HB2	2.41	0.51
2:H:106:GLY:O	2:H:111:GLY:HA3	2.11	0.50
2:F:50:ASN:O	2:F:64:ARG:NH2	2.38	0.50
2:H:139:HIS:HD2	2:H:146:GLY:O	1.94	0.50
2:F:6:HIS:CE1	2:F:8:GLN:HG3	2.46	0.50
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.46	0.50
2:F:282:GLN:CB	2:F:283:TYR:HA	2.41	0.50
2:F:407:TRP:CH2	1:G:256:GLN:HB3	2.47	0.50
2:F:106:GLY:O	2:F:111:GLY:HA3	2.11	0.49
2:D:331:GLN:O	2:D:335:VAL:HG23	2.12	0.49
3:I:116:PHE:HA	3:I:119:MET:HB2	1.94	0.49
2:H:325:MET:CE	2:H:355:VAL:HG11	2.42	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.49
2:D:106:GLY:O	2:D:111:GLY:HA3	2.11	0.49
1:G:107:HIS:HE1	1:G:155:GLU:OE2	1.95	0.49
2:B:331:GLN:O	2:B:335:VAL:HG23	2.13	0.49
1:E:107:HIS:HE1	1:E:155:GLU:OE2	1.95	0.49
2:B:101:ASN:HB3	2:B:180:THR:HG21	1.95	0.49
1:E:246:GLY:H	1:E:249:ASN:HD21	1.61	0.49
1:G:209:ILE:HD11	1:G:302:MET:CE	2.43	0.49
3:I:179:GLU:O	3:I:183:GLU:HB2	2.11	0.49
2:F:331:GLN:O	2:F:335:VAL:HG23	2.12	0.49
2:H:133:GLN:NE2	2:H:252:LEU:H	2.10	0.49
2:H:69:ASP:HB3	2:H:94:PHE:HD1	1.78	0.48
2:B:414:ASP:HB2	3:I:85:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.31	0.48
1:A:400:ALA:HB2	2:B:442:GLU:HG2	1.96	0.48
1:A:105:ARG:NE	1:A:110:ILE:HD11	2.27	0.48
2:F:269:MET:HE1	2:F:305:CYS:HB2	1.94	0.48
3:I:150:GLU:O	3:I:154:GLN:HB2	2.12	0.48
2:D:101:ASN:HB3	2:D:180:THR:HG21	1.95	0.48
2:H:325:MET:HE1	2:H:355:VAL:HG11	1.95	0.48
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.32	0.48
2:F:101:ASN:HB3	2:F:180:THR:HG21	1.96	0.47
2:H:178:SER:HB3	2:H:183:GLU:OE2	2.14	0.47
2:H:101:ASN:HB3	2:H:180:THR:HG21	1.96	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.47
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.96	0.47
2:F:156:LYS:HE2	3:I:178:ARG:HD2	1.96	0.47
2:F:6:HIS:CE1	2:F:8:GLN:HE21	2.33	0.47
2:H:88:ARG:NH1	2:H:90:ASP:OD1	2.47	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.97	0.47
3:I:97:ALA:HA	3:I:100:LYS:HB2	1.97	0.47
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.33	0.47
3:I:133:VAL:HG12	3:I:136:ARG:HH11	1.80	0.47
2:H:411:GLU:HA	3:I:239:LYS:HD3	1.97	0.46
2:F:123:ARG:O	2:F:127:GLU:HG2	2.15	0.46
3:I:227:GLU:C	3:I:229:ASP:H	2.19	0.46
2:D:286:LEU:HD13	2:D:290:GLU:HB3	1.97	0.46
2:H:92:PHE:CD2	2:H:94:PHE:HE2	2.30	0.46
3:I:182:ARG:HA	3:I:185:ILE:HB	1.97	0.46
2:H:385:GLN:HE22	2:H:433:GLN:HE21	1.63	0.46
1:A:352:LYS:HG2	3:I:21:GLU:HG3	1.98	0.46
2:H:323:MET:O	2:H:325:MET:HE3	2.15	0.46
1:G:167:LEU:HG	1:G:200:CYS:HB3	1.98	0.46
2:H:2:ARG:NH2	2:H:3:GLU:OE1	2.46	0.46
2:H:123:ARG:O	2:H:127:GLU:HG2	2.16	0.46
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.97	0.45
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.30	0.45
2:H:6:HIS:CE1	2:H:8:GLN:HE21	2.32	0.45
2:D:123:ARG:O	2:D:127:GLU:HG2	2.17	0.45
3:I:192:ASN:O	3:I:194:ASN:N	2.49	0.45
1:G:192:HIS:CG	1:G:421:ALA:HA	2.52	0.45
2:H:331:GLN:O	2:H:335:VAL:HG23	2.17	0.45
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.32	0.45
1:G:209:ILE:HD11	1:G:302:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:NE2	1:A:372:GLN:H	2.14	0.45
1:A:261:PRO:HG3	1:A:313:MET:HG3	1.98	0.45
1:G:107:HIS:NE2	3:I:206:LYS:HE3	2.32	0.45
3:I:56:ALA:HB1	3:I:60:ARG:NH1	2.31	0.45
1:G:209:ILE:HG22	1:G:227:LEU:HD22	1.99	0.44
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.57	0.44
1:G:411:GLU:C	3:I:214:ARG:HG3	2.37	0.44
2:F:83:PHE:O	2:F:86:ILE:HG22	2.17	0.44
2:F:345:GLU:H	2:F:345:GLU:HG2	1.55	0.44
2:B:269:MET:HE1	2:B:305:CYS:HB2	1.99	0.44
1:E:209:ILE:HG22	1:E:227:LEU:HD22	1.99	0.44
2:D:288:VAL:HG22	2:D:323:MET:HE3	1.99	0.44
1:E:167:LEU:HG	1:E:200:CYS:HB3	1.98	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.44
2:F:312:TYR:CE2	2:F:377:PHE:HZ	2.35	0.44
2:H:288:VAL:HG22	2:H:323:MET:HE3	2.00	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.44
1:E:209:ILE:HD11	1:E:302:MET:SD	2.58	0.44
2:D:407:TRP:CH2	1:E:256:GLN:HB3	2.53	0.44
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.99	0.43
2:D:229:HIS:CE1	2:D:276:THR:HG23	2.51	0.43
2:B:286:LEU:HD13	2:B:290:GLU:HB3	2.00	0.43
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.43
2:D:269:MET:HE1	2:D:305:CYS:HB2	2.00	0.43
2:F:12:CYS:HB3	2:F:140:SER:HB3	2.00	0.43
3:I:220:ALA:O	3:I:224:ARG:HD3	2.18	0.43
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.53	0.43
1:C:209:ILE:HD11	1:C:302:MET:CE	2.49	0.43
2:D:2:ARG:HB2	2:D:2:ARG:NH1	2.33	0.43
3:I:218:PHE:HA	3:I:221:MET:HB3	2.01	0.43
3:I:192:ASN:C	3:I:194:ASN:N	2.71	0.43
2:F:66:ILE:HG12	2:F:121:VAL:HG12	2.01	0.43
1:C:217:LEU:HD21	1:C:368:LEU:HD23	2.00	0.43
1:G:88:HIS:O	1:G:91:GLN:HG2	2.18	0.43
1:E:88:HIS:O	1:E:91:GLN:HG2	2.18	0.43
1:E:209:ILE:HD11	1:E:302:MET:CE	2.49	0.43
2:B:123:ARG:O	2:B:127:GLU:HG2	2.18	0.43
1:G:217:LEU:HD21	1:G:368:LEU:HD23	2.00	0.43
2:H:292:THR:CG2	2:H:335:VAL:HG21	2.41	0.43
3:I:182:ARG:O	3:I:186:GLN:HG3	2.17	0.43
1:E:97:GLU:HG3	2:F:1:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:130:ALA:O	3:I:134:ARG:HB2	2.19	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.42
1:E:217:LEU:HD21	1:E:368:LEU:HD23	2.00	0.42
2:H:171:VAL:HA	2:H:204:ILE:O	2.19	0.42
2:H:312:TYR:CE2	2:H:377:PHE:HZ	2.37	0.42
2:F:286:LEU:HD13	2:F:290:GLU:HB3	2.00	0.42
2:H:133:GLN:HB3	2:H:133:GLN:HE21	1.31	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:C:12:ALA:CB	1:C:140:SER:HB3	2.50	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.42
2:D:239:THR:O	2:D:243:ARG:HG2	2.20	0.42
1:E:192:HIS:CG	1:E:421:ALA:HA	2.55	0.42
2:H:92:PHE:HD2	2:H:94:PHE:CE2	2.34	0.42
2:B:414:ASP:HB2	3:I:85:ARG:NH2	2.34	0.42
2:H:269:MET:HG3	2:H:303:ALA:HB3	2.00	0.42
1:A:311:LYS:HG2	1:A:342:GLN:HG2	2.02	0.42
1:G:12:ALA:CB	1:G:140:SER:HB3	2.49	0.42
2:H:83:PHE:O	2:H:86:ILE:HG22	2.19	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.42
1:C:141:PHE:CE2	1:C:170:SER:HB3	2.55	0.42
3:I:32:VAL:HB	3:I:33:PRO:HD2	2.00	0.42
1:G:141:PHE:O	1:G:147:SER:HB3	2.20	0.42
2:F:385:GLN:HE22	2:F:433:GLN:HE21	1.67	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:F:2:ARG:HB2	2:F:2:ARG:NH1	2.34	0.42
3:I:134:ARG:HA	3:I:134:ARG:HD2	1.91	0.42
2:B:269:MET:HE3	2:B:305:CYS:HB2	2.02	0.42
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.42
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.54	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.41
2:D:220:THR:HB	1:E:326:LYS:HE3	2.02	0.41
1:C:88:HIS:H	1:C:91:GLN:NE2	2.19	0.41
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.01	0.41
1:E:12:ALA:CB	1:E:140:SER:HB3	2.50	0.41
1:E:250:VAL:CG2	1:E:255:PHE:CD1	2.99	0.41
1:E:88:HIS:H	1:E:91:GLN:NE2	2.18	0.41
1:C:36:MET:HA	1:C:37:PRO:HD3	1.97	0.41
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.03	0.41
2:F:171:VAL:HA	2:F:204:ILE:O	2.20	0.41
2:F:412:GLY:O	3:I:187:ARG:NH1	2.53	0.41
1:C:347:CYS:HA	1:C:348:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ILE:HG12	2:B:121:VAL:HG12	2.03	0.41
2:B:181:VAL:HA	1:C:349:THR:CG2	2.50	0.41
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.02	0.41
3:I:157:GLU:HG3	3:I:161:GLU:OE1	2.20	0.41
1:C:271:THR:HG22	1:C:301:GLN:HA	2.03	0.41
2:H:12:CYS:HB3	2:H:140:SER:HB3	2.02	0.41
1:E:320:ARG:HG3	1:E:360:PRO:HD3	2.03	0.41
3:I:6:MET:SD	3:I:22:VAL:HG13	2.61	0.41
1:C:271:THR:OG1	1:C:377:MET:HB3	2.21	0.41
2:H:66:ILE:HG12	2:H:121:VAL:HG12	2.01	0.41
2:B:83:PHE:O	2:B:86:ILE:HG22	2.20	0.41
2:B:220:THR:HB	1:C:326:LYS:HE3	2.02	0.41
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.40
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.68	0.40
1:G:320:ARG:HG3	1:G:360:PRO:HD3	2.03	0.40
1:A:12:ALA:CB	1:A:140:SER:HB3	2.52	0.40
1:C:88:HIS:O	1:C:91:GLN:HG2	2.22	0.40
2:D:345:GLU:H	2:D:345:GLU:HG2	1.58	0.40
2:F:239:THR:O	2:F:243:ARG:HG2	2.22	0.40
2:H:239:THR:O	2:H:243:ARG:HG2	2.21	0.40
2:F:79:ARG:HH22	2:F:94:PHE:HE2	1.69	0.40
1:G:119:LEU:HD11	1:G:156:ARG:HB3	2.02	0.40
1:G:347:CYS:HA	1:G:348:PRO:HD3	1.94	0.40
2:H:295:MET:HG3	2:H:377:PHE:HD1	1.86	0.40
1:A:209:ILE:HD11	1:A:302:MET:CE	2.51	0.40
1:A:355:ILE:HD11	3:I:20:TRP:HH2	1.87	0.40
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.03	0.40
1:G:210:TYR:CZ	1:G:222:PRO:HD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ALA:CB	2:H:89:PRO:O[2_556]	2.04	0.16

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	427/451 (95%)	410 (96%)	15 (4%)	2 (0%)	34	77
1	C	427/451 (95%)	405 (95%)	17 (4%)	5 (1%)	16	62
1	E	427/451 (95%)	406 (95%)	16 (4%)	5 (1%)	16	62
1	G	427/451 (95%)	405 (95%)	17 (4%)	5 (1%)	16	62
2	B	430/445 (97%)	413 (96%)	15 (4%)	2 (0%)	34	77
2	D	430/445 (97%)	413 (96%)	14 (3%)	3 (1%)	26	71
2	F	430/445 (97%)	412 (96%)	15 (4%)	3 (1%)	26	71
2	H	429/445 (96%)	412 (96%)	14 (3%)	3 (1%)	26	71
3	I	230/240 (96%)	192 (84%)	32 (14%)	6 (3%)	7	48
All	All	3657/3824 (96%)	3468 (95%)	155 (4%)	34 (1%)	21	67

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	282	GLN
1	C	348	PRO
2	D	282	GLN
1	E	348	PRO
2	F	282	GLN
1	G	348	PRO
1	A	47	ASP
1	A	437	VAL
1	C	47	ASP
1	C	339	ARG
1	E	47	ASP
1	E	339	ARG
1	G	47	ASP
1	G	339	ARG
2	H	98	GLY
3	I	193	ASN

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Mol	Chain	Res	Type
1	C	280	LYS
1	E	280	LYS
1	G	280	LYS
2	H	280	SER
1	C	283	HIS
2	D	280	SER
2	D	284	ARG
1	E	283	HIS
1	G	283	HIS
3	I	35	PHE
2	B	284	ARG
2	F	280	SER
2	F	284	ARG
2	H	278	ARG
3	I	30	ASP
3	I	96	MET
3	I	97	ALA
3	I	44	ASP

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	365/379 (96%)	348 (95%)	17 (5%)	32 70
1	C	359/379 (95%)	342 (95%)	17 (5%)	32 70
1	E	359/379 (95%)	343 (96%)	16 (4%)	34 71
1	G	359/379 (95%)	342 (95%)	17 (5%)	32 70
2	B	369/383 (96%)	358 (97%)	11 (3%)	48 79
2	D	369/383 (96%)	358 (97%)	11 (3%)	48 79
2	F	369/383 (96%)	358 (97%)	11 (3%)	48 79
2	H	369/383 (96%)	353 (96%)	16 (4%)	35 72
3	I	198/212 (93%)	165 (83%)	33 (17%)	3 21
All	All	3116/3260 (96%)	2967 (95%)	149 (5%)	31 70

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	4	CYS
1	A	46	ASP
1	A	73	THR
1	A	84	ARG
1	A	113	GLU
1	A	163	LYS
1	A	215	ARG
1	A	250	VAL
1	A	316	CYS
1	A	324	VAL
1	A	345	ASP
1	A	358	GLN
1	A	370	LYS
1	A	414	GLU
1	A	434	GLU
2	B	115	VAL
2	B	122	VAL
2	B	128	SER
2	B	158	ARG
2	B	171	VAL
2	B	178	SER
2	B	241	CYS
2	B	298	SER
2	B	325	MET
2	B	341	SER
2	B	377	PHE
1	C	1	MET
1	C	4	CYS
1	C	46	ASP
1	C	62	VAL
1	C	73	THR
1	C	84	ARG
1	C	127	ASP
1	C	164	LYS
1	C	241	SER
1	C	250	VAL
1	C	271	THR
1	C	316	CYS
1	C	324	VAL
1	C	339	ARG

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Mol	Chain	Res	Type
1	C	340	SER
1	C	414	GLU
1	C	430	LYS
2	D	115	VAL
2	D	128	SER
2	D	158	ARG
2	D	171	VAL
2	D	178	SER
2	D	181	VAL
2	D	241	CYS
2	D	298	SER
2	D	325	MET
2	D	341	SER
2	D	377	PHE
1	E	1	MET
1	E	4	CYS
1	E	62	VAL
1	E	73	THR
1	E	84	ARG
1	E	127	ASP
1	E	164	LYS
1	E	241	SER
1	E	250	VAL
1	E	271	THR
1	E	316	CYS
1	E	324	VAL
1	E	339	ARG
1	E	340	SER
1	E	414	GLU
1	E	430	LYS
2	F	122	VAL
2	F	128	SER
2	F	158	ARG
2	F	171	VAL
2	F	178	SER
2	F	241	CYS
2	F	298	SER
2	F	325	MET
2	F	341	SER
2	F	377	PHE
2	F	442	GLU
1	G	1	MET

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Mol	Chain	Res	Type
1	G	4	CYS
1	G	46	ASP
1	G	62	VAL
1	G	73	THR
1	G	84	ARG
1	G	127	ASP
1	G	241	SER
1	G	250	VAL
1	G	271	THR
1	G	316	CYS
1	G	324	VAL
1	G	339	ARG
1	G	340	SER
1	G	401	LYS
1	G	414	GLU
1	G	430	LYS
2	H	115	VAL
2	H	122	VAL
2	H	128	SER
2	H	147	SER
2	H	158	ARG
2	H	171	VAL
2	H	179	ASP
2	H	241	CYS
2	H	276	THR
2	H	284	ARG
2	H	286	LEU
2	H	295	MET
2	H	325	MET
2	H	341	SER
2	H	377	PHE
2	H	406	HIS
3	I	5	ASP
3	I	21	GLU
3	I	29	PHE
3	I	49	GLU
3	I	50	ILE
3	I	52	LYS
3	I	53	LYS
3	I	54	LEU
3	I	100	LYS
3	I	113	GLU

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Mol	Chain	Res	Type
3	I	120	LEU
3	I	125	GLU
3	I	145	ILE
3	I	150	GLU
3	I	152	LEU
3	I	158	SER
3	I	163	ARG
3	I	166	GLN
3	I	172	LYS
3	I	177	LYS
3	I	201	GLU
3	I	203	LEU
3	I	208	GLU
3	I	221	MET
3	I	222	LEU
3	I	223	GLU
3	I	225	LEU
3	I	227	GLU
3	I	229	ASP
3	I	236	ARG
3	I	240	GLU
3	I	241	LEU
3	I	242	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	91	GLN
1	A	107	HIS
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	358	GLN
1	A	372	GLN
2	B	6	HIS
2	B	8	GLN

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Mol	Chain	Res	Type
2	B	14	ASN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	309	HIS
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	15	GLN
1	C	91	GLN
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
1	C	358	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	136	GLN
2	D	139	HIS
2	D	206	ASN
2	D	229	HIS
2	D	266	HIS
2	D	309	HIS
2	D	385	GLN
2	D	433	GLN
1	E	8	HIS
1	E	15	GLN
1	E	91	GLN
1	E	107	HIS
1	E	133	GLN
1	E	139	HIS
1	E	197	HIS
1	E	249	ASN
1	E	301	GLN
1	E	358	GLN
2	F	6	HIS
2	F	8	GLN
2	F	14	ASN
2	F	139	HIS

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Mol	Chain	Res	Type
2	F	206	ASN
2	F	229	HIS
2	F	266	HIS
2	F	309	HIS
2	F	385	GLN
2	F	433	GLN
1	G	8	HIS
1	G	15	GLN
1	G	91	GLN
1	G	107	HIS
1	G	133	GLN
1	G	139	HIS
1	G	197	HIS
1	G	249	ASN
1	G	301	GLN
1	G	329	ASN
1	G	358	GLN
2	H	6	HIS
2	H	8	GLN
2	H	14	ASN
2	H	133	GLN
2	H	139	HIS
2	H	206	ASN
2	H	247	GLN
2	H	266	HIS
2	H	385	GLN
2	H	433	GLN
3	I	205	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	GTP	A	600	5	25,34,34	1.08	2 (8%)	34,54,54	1.99	5 (14%)
6	GDP	B	600	-	23,30,30	1.08	1 (4%)	30,47,47	2.10	4 (13%)
4	GTP	C	600	5	25,34,34	1.06	2 (8%)	34,54,54	2.00	5 (14%)
6	GDP	D	600	-	23,30,30	1.18	3 (13%)	30,47,47	2.12	6 (20%)
4	GTP	E	600	5	25,34,34	1.10	2 (8%)	34,54,54	2.07	5 (14%)
6	GDP	F	600	-	23,30,30	1.04	2 (8%)	30,47,47	2.15	4 (13%)
4	GTP	G	600	5	25,34,34	0.97	2 (8%)	34,54,54	2.07	5 (14%)
6	GDP	H	600	-	23,30,30	1.02	2 (8%)	30,47,47	2.20	4 (13%)

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
4	GTP	A	600	5	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
4	GTP	C	600	5	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3
4	GTP	E	600	5	-	0/18/38/38	0/3/3/3
6	GDP	F	600	-	-	0/12/32/32	0/3/3/3
4	GTP	G	600	5	-	0/18/38/38	0/3/3/3
6	GDP	H	600	-	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	GDP	C6-C5	2.09	1.45	1.41
4	G	600	GTP	C6-C5	2.26	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	GDP	C6-C5	2.28	1.45	1.41
6	H	600	GDP	PB-O2B	2.32	1.63	1.54
4	G	600	GTP	C6-N1	2.75	1.38	1.33
4	C	600	GTP	C6-C5	2.91	1.47	1.41
6	D	600	GDP	PB-O1B	2.92	1.60	1.51
4	A	600	GTP	C6-N1	2.93	1.38	1.33
4	C	600	GTP	C6-N1	2.94	1.38	1.33
4	E	600	GTP	C6-N1	2.95	1.38	1.33
4	A	600	GTP	C6-C5	3.05	1.47	1.41
6	D	600	GDP	C6-N1	3.16	1.39	1.33
4	E	600	GTP	C6-C5	3.17	1.47	1.41
6	H	600	GDP	C6-N1	3.27	1.39	1.33
6	F	600	GDP	C6-N1	3.27	1.39	1.33
6	B	600	GDP	C6-N1	3.60	1.39	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	600	GDP	C5-C6-N1	-8.23	112.34	123.59
4	E	600	GTP	C5-C6-N1	-8.23	112.34	123.59
4	G	600	GTP	C5-C6-N1	-8.18	112.40	123.59
6	F	600	GDP	C5-C6-N1	-8.18	112.41	123.59
4	A	600	GTP	C5-C6-N1	-7.91	112.78	123.59
4	C	600	GTP	C5-C6-N1	-7.89	112.80	123.59
6	B	600	GDP	C5-C6-N1	-7.89	112.81	123.59
6	D	600	GDP	C5-C6-N1	-7.77	112.96	123.59
4	C	600	GTP	C6-C5-C4	-2.99	117.32	120.90
4	A	600	GTP	C6-C5-C4	-2.91	117.42	120.90
4	E	600	GTP	C6-C5-C4	-2.89	117.44	120.90
6	B	600	GDP	N3-C2-N1	-2.78	123.21	127.44
6	D	600	GDP	N3-C2-N1	-2.71	123.32	127.44
4	G	600	GTP	C6-C5-C4	-2.68	117.70	120.90
6	D	600	GDP	C6-C5-C4	-2.67	117.70	120.90
6	H	600	GDP	N3-C2-N1	-2.66	123.39	127.44
6	F	600	GDP	N3-C2-N1	-2.65	123.40	127.44
4	C	600	GTP	N3-C2-N1	-2.61	123.47	127.44
6	B	600	GDP	C6-C5-C4	-2.59	117.80	120.90
4	G	600	GTP	N3-C2-N1	-2.51	123.62	127.44
4	A	600	GTP	N3-C2-N1	-2.49	123.66	127.44
6	F	600	GDP	C6-C5-C4	-2.44	117.99	120.90
4	E	600	GTP	N3-C2-N1	-2.43	123.74	127.44
6	H	600	GDP	C6-C5-C4	-2.14	118.34	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	600	GDP	O2B-PB-O1B	2.04	117.16	110.58
6	D	600	GDP	C2'-C1'-N9	2.05	117.43	114.29
4	C	600	GTP	O3A-PA-O5'	2.24	108.87	102.94
4	A	600	GTP	O3A-PA-O5'	2.27	108.95	102.94
4	G	600	GTP	O3A-PA-O5'	2.63	109.91	102.94
4	E	600	GTP	O3A-PA-O5'	2.69	110.06	102.94
4	A	600	GTP	C6-N1-C2	6.41	124.83	115.94
6	D	600	GDP	C6-N1-C2	6.52	124.99	115.94
4	C	600	GTP	C6-N1-C2	6.54	125.01	115.94
6	B	600	GDP	C6-N1-C2	6.57	125.06	115.94
4	G	600	GTP	C6-N1-C2	6.64	125.15	115.94
6	H	600	GDP	C6-N1-C2	6.65	125.17	115.94
6	F	600	GDP	C6-N1-C2	6.68	125.21	115.94
4	E	600	GTP	C6-N1-C2	6.71	125.25	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	600	GDP	1	0
6	D	600	GDP	1	0
6	F	600	GDP	1	0
6	H	600	GDP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	431/451 (95%)	0.23	24 (5%) 28 20	95, 145, 234, 287	0
1	C	431/451 (95%)	0.54	41 (9%) 10 8	154, 217, 276, 289	0
1	E	431/451 (95%)	0.40	35 (8%) 15 11	164, 208, 281, 287	0
1	G	431/451 (95%)	0.28	22 (5%) 32 24	99, 149, 278, 291	0
2	B	432/445 (97%)	0.32	21 (4%) 33 25	95, 150, 261, 300	0
2	D	432/445 (97%)	0.49	38 (8%) 12 9	158, 211, 281, 284	0
2	F	432/445 (97%)	0.34	25 (5%) 26 19	147, 187, 282, 291	0
2	H	431/445 (96%)	0.05	10 (2%) 64 53	71, 116, 178, 274	0
3	I	234/240 (97%)	0.31	9 (3%) 44 34	108, 193, 273, 291	0
All	All	3685/3824 (96%)	0.33	225 (6%) 25 17	71, 177, 278, 300	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	442	GLU	7.0
2	D	323	MET	7.0
3	I	4	ALA	6.8
1	G	46	ASP	6.3
2	F	442	GLU	6.1
1	G	283	HIS	6.0
2	D	284	ARG	5.7
2	D	28	HIS	5.6
1	C	370	LYS	5.2
1	E	281	ALA	5.0
2	F	37	HIS	4.9
1	E	46	ASP	4.8
1	C	46	ASP	4.8
1	A	436	GLY	4.8
2	B	61	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	43	GLN	4.6
1	A	247	ALA	4.5
2	F	283	TYR	4.5
1	G	284	GLU	4.5
1	A	313	MET	4.3
2	D	41	ASP	4.3
1	C	274	PRO	4.3
1	C	283	HIS	4.2
2	D	369	ARG	4.2
1	A	284	GLU	4.1
1	A	435	VAL	4.1
2	D	246	GLY	4.1
2	D	220	THR	4.1
1	G	309	HIS	4.1
1	G	346	TRP	4.0
1	C	29	GLY	4.0
1	A	283	HIS	4.0
2	D	37	HIS	4.0
1	C	244	PHE	3.9
1	E	280	LYS	3.9
1	E	49	PHE	3.8
1	C	371	VAL	3.8
1	A	438	ASP	3.7
1	E	323	VAL	3.7
2	B	59	ASN	3.7
1	E	283	HIS	3.7
2	B	438	ALA	3.7
1	C	367	ASP	3.7
1	C	323	VAL	3.6
2	F	284	ARG	3.5
2	D	373	MET	3.4
2	B	288	VAL	3.4
1	G	308	ARG	3.4
3	I	33	PRO	3.3
1	A	281	ALA	3.3
1	C	28	HIS	3.3
2	D	83	PHE	3.3
1	E	36	MET	3.2
2	F	61	TYR	3.2
1	E	47	ASP	3.2
1	G	342	GLN	3.1
1	A	280	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	286	LEU	3.1
2	D	372	LYS	3.1
2	H	440	ALA	3.1
1	C	161	TYR	3.1
1	A	311	LYS	3.1
2	D	283	TYR	3.1
1	C	320	ARG	3.0
1	A	1	MET	3.0
2	D	61	TYR	3.0
2	F	159	GLU	3.0
1	E	373	ARG	3.0
1	C	361	THR	3.0
2	D	408	TYR	3.0
2	D	324	SER	3.0
3	I	113	GLU	3.0
1	E	346	TRP	3.0
2	D	222	PRO	2.9
2	H	441	ASP	2.9
1	E	395	PHE	2.9
2	F	30	ILE	2.9
2	D	442	GLU	2.9
2	B	440	ALA	2.9
1	A	437	VAL	2.9
2	H	61	TYR	2.9
2	D	358	ILE	2.9
1	E	61	HIS	2.8
1	C	25	CYS	2.8
2	B	243	ARG	2.8
1	C	162	GLY	2.8
1	G	47	ASP	2.8
1	E	30	ILE	2.8
1	G	245	ASP	2.8
2	F	305	CYS	2.8
2	B	441	ASP	2.8
1	C	285	GLN	2.8
2	D	39	ASP	2.8
1	A	285	GLN	2.8
1	C	30	ILE	2.8
1	G	30	ILE	2.8
2	D	40	SER	2.8
2	F	32	PRO	2.8
2	F	346	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	180	ALA	2.7
2	B	30	ILE	2.7
2	D	38	GLY	2.7
2	F	98	GLY	2.7
1	E	156	ARG	2.7
2	D	371	LEU	2.7
2	B	83	PHE	2.7
1	C	83	TYR	2.7
3	I	32	VAL	2.7
2	B	98	GLY	2.6
1	C	37	PRO	2.6
2	F	282	GLN	2.6
1	C	340	SER	2.6
2	B	326	LYS	2.6
2	D	418	PHE	2.6
2	D	59	ASN	2.6
2	B	281	GLN	2.6
1	E	341	ILE	2.6
2	H	57	THR	2.6
1	C	36	MET	2.6
2	D	219	LEU	2.6
1	G	280	LYS	2.6
1	C	319	TYR	2.6
2	H	306	ASP	2.6
1	C	245	ASP	2.5
1	C	1	MET	2.5
2	F	38	GLY	2.5
1	A	2	ARG	2.5
1	E	355	ILE	2.5
1	G	37	PRO	2.5
1	G	36	MET	2.5
1	A	349	THR	2.5
1	E	340	SER	2.5
1	A	344	VAL	2.5
1	E	197	HIS	2.5
1	C	362	VAL	2.4
1	E	282	TYR	2.4
1	G	156	ARG	2.4
1	C	97	GLU	2.4
1	C	170	SER	2.4
2	F	220	THR	2.4
2	B	279	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	246	GLY	2.4
1	A	46	ASP	2.4
1	A	345	ASP	2.4
2	H	176	LYS	2.4
1	G	249	ASN	2.4
1	E	296	PHE	2.4
2	B	323	MET	2.4
1	A	355	ILE	2.4
1	G	1	MET	2.4
1	G	281	ALA	2.4
1	E	397	LEU	2.4
2	F	36	TYR	2.3
1	E	277	SER	2.3
2	F	299	LYS	2.3
2	F	218	LYS	2.3
2	B	319	PHE	2.3
2	D	279	GLY	2.3
3	I	111	ASN	2.3
1	E	418	PHE	2.3
2	H	309	HIS	2.3
1	C	356	ASN	2.3
1	C	299	ALA	2.3
2	D	32	PRO	2.3
2	F	178	SER	2.3
1	C	284	GLU	2.3
2	D	440	ALA	2.3
2	B	57	THR	2.3
1	A	382	THR	2.3
1	G	58	ALA	2.3
2	F	111	GLY	2.3
1	C	241	SER	2.3
3	I	24	LEU	2.3
2	H	142	GLY	2.3
1	G	306	ASP	2.3
1	E	252	LEU	2.2
1	G	33	ASP	2.2
2	D	360	PRO	2.2
1	A	170	SER	2.2
2	B	44	LEU	2.2
1	E	413	MET	2.2
2	D	214	PHE	2.2
1	E	58	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	2.2
1	E	32	PRO	2.2
3	I	190	GLU	2.2
1	A	343	PHE	2.2
1	C	26	LEU	2.2
3	I	5	ASP	2.2
1	E	135	PHE	2.2
1	C	386	GLU	2.2
2	D	374	SER	2.2
1	C	398	MET	2.2
1	C	288	VAL	2.1
2	F	100	GLY	2.1
1	E	50	ASN	2.1
1	E	247	ALA	2.1
2	F	216	THR	2.1
1	A	401	LYS	2.1
1	C	31	GLN	2.1
1	E	35	GLN	2.1
1	G	246	GLY	2.1
2	D	327	GLU	2.1
2	F	108	TYR	2.1
2	B	37	HIS	2.1
1	E	69	ASP	2.1
1	E	34	GLY	2.1
2	B	36	TYR	2.1
2	D	65	ALA	2.1
2	F	86	ILE	2.1
1	C	363	VAL	2.1
1	E	322	ASP	2.1
2	B	346	TRP	2.1
1	C	360	PRO	2.1
1	G	285	GLN	2.1
2	D	221	THR	2.1
2	H	439	THR	2.1
1	C	27	GLU	2.1
1	E	60	LYS	2.1
2	F	156	LYS	2.1
2	F	400	ARG	2.0
2	D	379	GLY	2.0
3	I	19	SER	2.0
2	D	215	ARG	2.0
2	D	322	ARG	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
6	GDP	F	600	28/28	0.83	0.44	0.57	153,157,163,165	0
6	GDP	B	600	28/28	0.86	0.37	0.28	117,126,131,134	0
6	GDP	D	600	28/28	0.78	0.35	0.13	175,181,190,195	0
4	GTP	C	600	32/32	0.87	0.34	-0.03	169,176,188,193	0
4	GTP	A	600	32/32	0.90	0.31	-0.22	99,105,112,115	0
4	GTP	G	600	32/32	0.91	0.30	-0.57	100,104,115,116	0
6	GDP	H	600	28/28	0.88	0.28	-0.62	85,92,96,99	0
4	GTP	E	600	32/32	0.94	0.25	-0.62	168,174,185,188	0
5	MG	A	601	1/1	0.88	0.35	-	102,102,102,102	0
5	MG	G	601	1/1	0.89	0.42	-	105,105,105,105	0
5	MG	E	601	1/1	0.96	0.37	-	175,175,175,175	0
5	MG	C	601	1/1	0.92	0.45	-	181,181,181,181	0

6.5 Other polymers (i)

There are no such residues in this entry.