Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 05:42 PM EDT

PDB ID	:	6GK4
Title	:	Human NBD1 of CFTR in complex with nanobodies D12 and T8
Authors	:	Sigoillot, M.; Overtus, M.; Grodecka, M.; Scholl, D.; Garcia-Pino, A.; Laeremans, T.; He, L.; Pardon, E.; Hildebrandt, E.; Urbatsch, I.; Steyaert, J.; Riordan, J.R.; Govaerts, C.
Deposited on	:	2018-05-18
Resolution	:	2.91 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

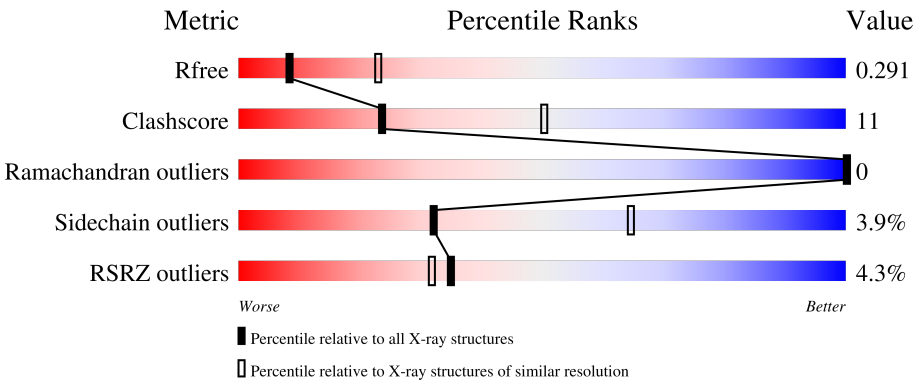
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.91 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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	229	5% 73% 17% • 8%
1	D	229	5% 72% 20% 8%
2	B	149	2% 68% 11% • 19%
2	E	149	2% 69% 13% 18%

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Mol	Chain	Length	Quality of chain
3	C	143	6% 64% 15% • 20%
3	F	143	60% 20% • 19%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6870 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	1586	1019	257	299	11	0	0	0
1	D	211	1537	993	246	287	11	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	SER	-	expression tag	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	GLY	deletion	UNP Q20BJ8
A	?	-	GLU	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	GLU	deletion	UNP Q20BJ8
A	?	-	LYS	deletion	UNP Q20BJ8
A	?	-	ALA	deletion	UNP Q20BJ8
A	?	-	LYS	deletion	UNP Q20BJ8
A	?	-	GLN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ARG	deletion	UNP Q20BJ8
A	?	-	LYS	deletion	UNP Q20BJ8
A	?	-	THR	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	GLY	deletion	UNP Q20BJ8
A	?	-	ASP	deletion	UNP Q20BJ8
A	?	-	ASP	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
D	386	SER	-	expression tag	UNP Q20BJ8
D	?	-	PHE	deletion	UNP Q20BJ8
D	?	-	GLY	deletion	UNP Q20BJ8
D	?	-	GLU	deletion	UNP Q20BJ8
D	?	-	LEU	deletion	UNP Q20BJ8
D	?	-	PHE	deletion	UNP Q20BJ8
D	?	-	GLU	deletion	UNP Q20BJ8
D	?	-	LYS	deletion	UNP Q20BJ8
D	?	-	ALA	deletion	UNP Q20BJ8
D	?	-	LYS	deletion	UNP Q20BJ8
D	?	-	GLN	deletion	UNP Q20BJ8
D	?	-	ASN	deletion	UNP Q20BJ8
D	?	-	ASN	deletion	UNP Q20BJ8
D	?	-	ASN	deletion	UNP Q20BJ8
D	?	-	ASN	deletion	UNP Q20BJ8
D	?	-	ARG	deletion	UNP Q20BJ8
D	?	-	LYS	deletion	UNP Q20BJ8
D	?	-	THR	deletion	UNP Q20BJ8
D	?	-	SER	deletion	UNP Q20BJ8
D	?	-	ASN	deletion	UNP Q20BJ8
D	?	-	GLY	deletion	UNP Q20BJ8
D	?	-	ASP	deletion	UNP Q20BJ8
D	?	-	ASP	deletion	UNP Q20BJ8
D	?	-	SER	deletion	UNP Q20BJ8
D	?	-	LEU	deletion	UNP Q20BJ8
D	?	-	PHE	deletion	UNP Q20BJ8
D	?	-	PHE	deletion	UNP Q20BJ8
D	?	-	SER	deletion	UNP Q20BJ8
D	?	-	ASN	deletion	UNP Q20BJ8
D	?	-	PHE	deletion	UNP Q20BJ8
D	?	-	SER	deletion	UNP Q20BJ8
D	?	-	LEU	deletion	UNP Q20BJ8
D	?	-	LEU	deletion	UNP Q20BJ8

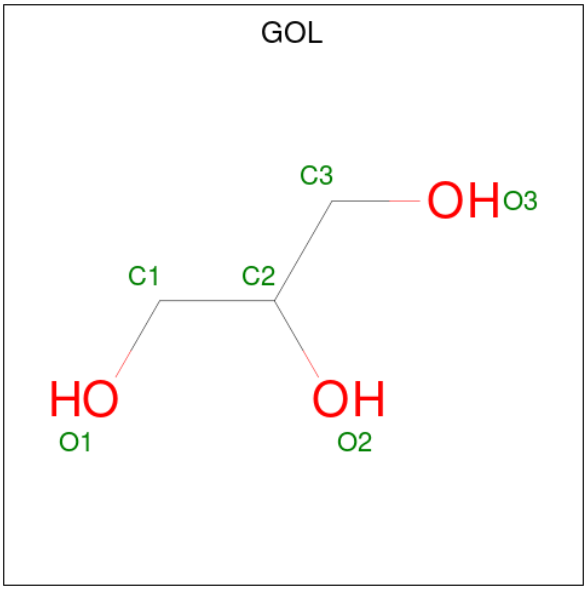
- Molecule 2 is a protein called Nanobody D12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	121	906	562	159	180	5	0	0	0
2	E	122	887	549	155	178	5	0	0	0

- Molecule 3 is a protein called Nanobody T8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	114	808	499	147	158	4	0	0	0
3	F	116	839	521	150	164	4	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

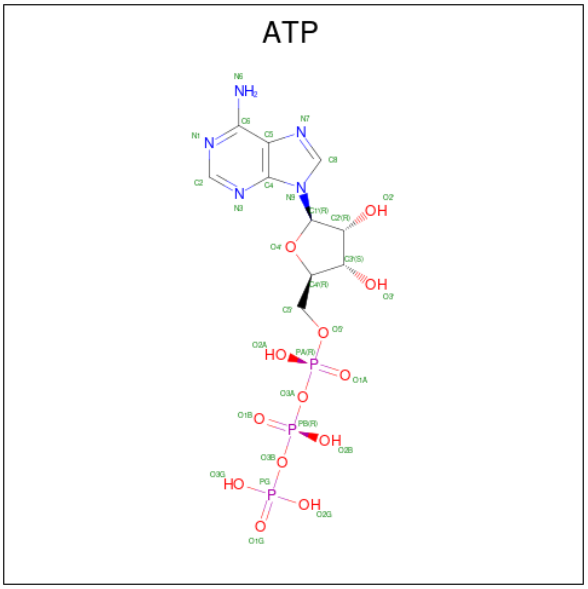


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	D	1	1	1	0	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
6	D	1	31	10	5	13	3	0	0

- Molecule 7 is water.

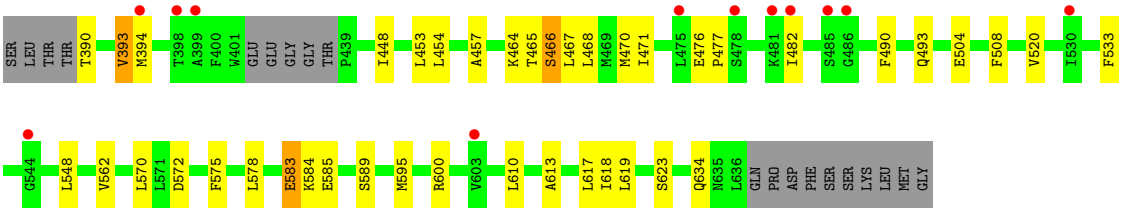
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	51	51	51	0	0
			Total	O		
7	B	25	25	25	0	0
			Total	O		
7	C	28	28	28	0	0
			Total	O		
7	D	46	46	46	0	0
			Total	O		
7	E	49	49	49	0	0
			Total	O		
7	F	38	38	38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

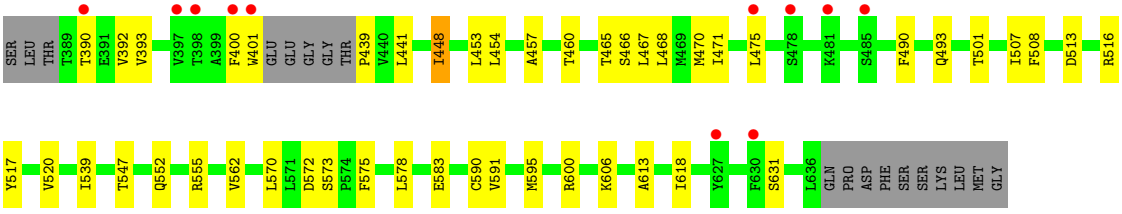
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain A:



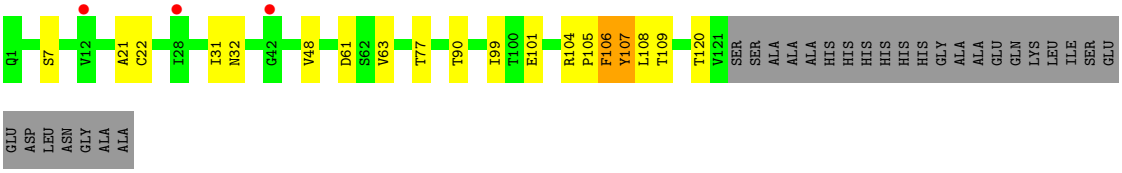
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain D:



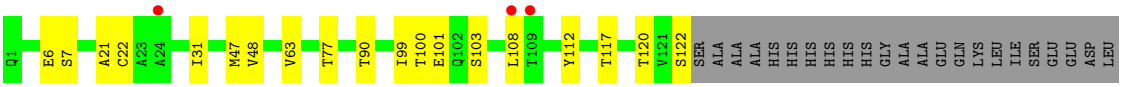
• Molecule 2: Nanobody D12

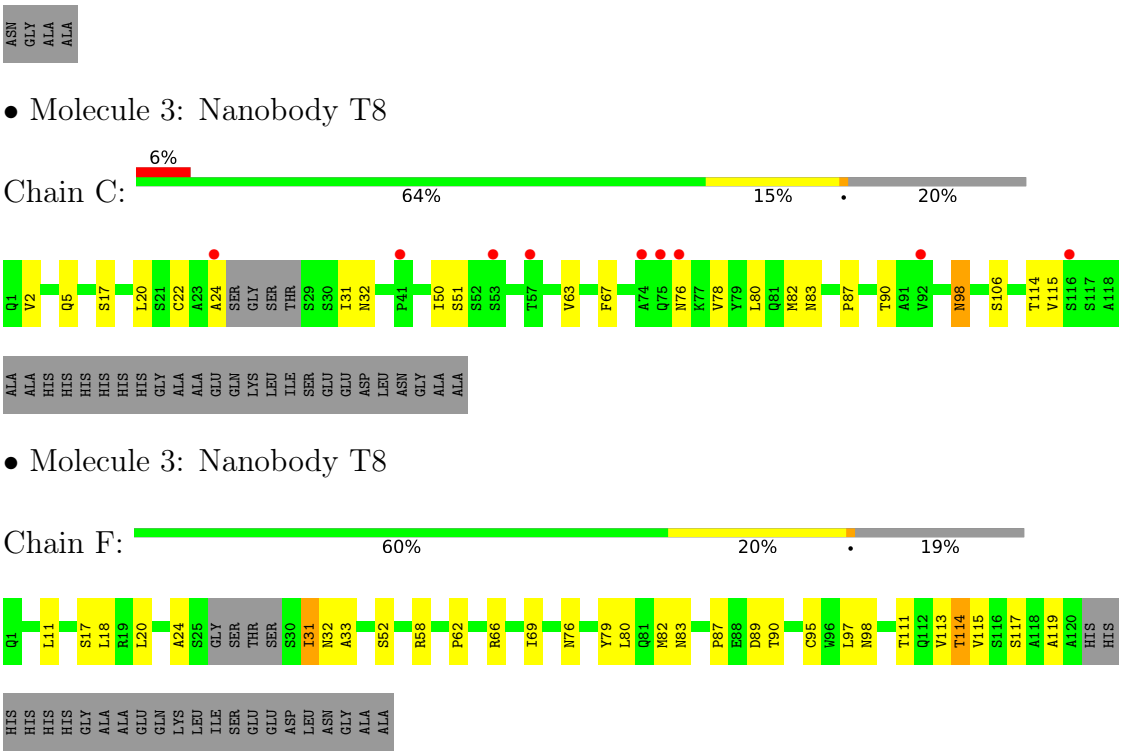
Chain B:



• Molecule 2: Nanobody D12

Chain E:




ASN GLY ALA ALA
• Molecule 3: Nanobody T8
Chain C:
6%
64%
15%
20%
Q1 V2 Q5 S17 L20 S21 C22 A23 A24 SER GLY SER THR S29 S30 I31 N32 P41 I50 S51 S52 S53 T57 V63 F67 A74 Q75 N76 K77 V78 Y79 L80 Q81 M82 N83 P87 T90 A91 V92 N98 S106 T114 V115 S116 S117 A118
ALA ALA HIS HIS HIS HIS HIS GLY ALA ALA GLU GLN LYS LEU ILE SER GLU GLU ASP LEU ASN GLY ALA ALA
• Molecule 3: Nanobody T8
Chain F:
60%
20%
19%
Q1 L11 S17 L18 R19 L20 A24 S25 GLY SER THR SER S30 I31 N32 A33 S52 R58 P62 R66 I69 N76 Y79 L80 Q81 M82 N83 P87 E88 D89 T90 C95 W96 L97 N98 T111 Q112 V113 T114 V115 S116 S117 A118 A119 A120 HIS HIS
HIS HIS HIS HIS GLY ALA ALA GLU GLN LYS LEU ILE SER GLU GLU ASP LEU ASN GLY ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.94Å 55.19Å 114.99Å 90.00° 103.96° 90.00°	Depositor
Resolution (Å)	45.16 – 2.91 45.16 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.16-2.91) 99.5 (45.16-2.91)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.246 , 0.295 0.248 , 0.291	Depositor DCC
R_{free} test set	1086 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 103.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% 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, 0.333 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: MG, GOL, ATP

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	0.57	0/1613	0.71	0/2180
1	D	0.57	0/1563	0.74	0/2117
2	B	0.48	0/922	0.72	0/1254
2	E	0.49	0/902	0.73	0/1229
3	C	0.55	0/825	0.73	0/1124
3	F	0.65	1/856 (0.1%)	0.76	0/1165
All	All	0.56	1/6681 (0.0%)	0.73	0/9069

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	95	CYS	N-CA	-5.28	1.35	1.46

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	1586	0	1534	37	0
1	D	1537	0	1444	39	0
2	B	906	0	853	13	0
2	E	887	0	816	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	808	0	708	22	0
3	F	839	0	773	31	0
4	A	6	0	8	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	31	0	12	5	0
6	D	31	0	12	6	0
7	A	51	0	0	0	0
7	B	25	0	0	0	0
7	C	28	0	0	0	0
7	D	46	0	0	0	0
7	E	49	0	0	0	0
7	F	38	0	0	0	0
All	All	6870	0	6160	143	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 11.

All (143) 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)
3:F:20:LEU:CD2	3:F:82:MET:CE	2.13	1.26
3:F:20:LEU:HD23	3:F:82:MET:CE	1.69	1.21
3:F:20:LEU:HD21	3:F:82:MET:HE1	1.31	1.11
3:F:20:LEU:HD23	3:F:82:MET:HE2	1.14	1.10
3:F:20:LEU:CD2	3:F:82:MET:HE1	1.80	1.10
3:F:20:LEU:CD2	3:F:82:MET:HE2	1.82	1.00
1:A:476:GLU:HG3	1:A:477:PRO:HD2	1.45	0.94
1:D:441:LEU:HD23	1:D:470:MET:HE2	1.48	0.94
1:D:392:VAL:CG1	1:D:448:ILE:HD12	2.04	0.87
2:B:101:GLU:N	2:B:101:GLU:OE2	2.07	0.86
1:A:465:THR:OG1	6:A:703:ATP:O1B	1.96	0.83
3:F:20:LEU:HD21	3:F:82:MET:CE	1.99	0.81
1:D:507:ILE:HD11	1:D:517:TYR:CD1	2.17	0.79
3:F:20:LEU:HD12	3:F:111:THR:HG21	1.63	0.79
1:D:591:VAL:O	1:D:600:ARG:NH1	2.16	0.78
1:A:470:MET:CE	1:A:482:ILE:HD11	2.12	0.77
3:C:67:PHE:CD1	3:C:82:MET:HA	2.21	0.76
1:A:465:THR:HG23	1:A:572:ASP:OD2	1.86	0.75
1:D:392:VAL:HG13	1:D:448:ILE:HD12	1.67	0.75
3:C:20:LEU:HG	3:C:82:MET:HE1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:OG	6:A:703:ATP:O1A	2.04	0.74
1:D:507:ILE:HD11	1:D:517:TYR:HD1	1.51	0.73
3:C:20:LEU:HG	3:C:82:MET:CE	2.18	0.72
1:A:470:MET:HE1	1:A:477:PRO:HB3	1.71	0.71
2:B:106:PHE:O	2:B:107:TYR:HB2	1.90	0.71
3:F:20:LEU:CD1	3:F:111:THR:HG21	2.19	0.71
1:A:465:THR:CB	6:A:703:ATP:O1B	2.41	0.69
2:B:104:ARG:HD3	2:B:106:PHE:HE1	1.59	0.67
1:D:562:VAL:HG11	1:D:590:CYS:SG	2.34	0.67
2:B:31:ILE:HG12	2:B:99:ILE:HG12	1.76	0.66
1:A:476:GLU:HG3	1:A:477:PRO:CD	2.24	0.64
1:A:390:THR:HG21	1:A:393:VAL:HG23	1.80	0.63
1:D:457:ALA:HB3	1:D:618:ILE:HG12	1.80	0.63
1:A:508:PHE:CD2	3:C:50:ILE:HD11	2.34	0.62
3:C:87:PRO:HA	3:C:115:VAL:HB	1.83	0.60
3:F:87:PRO:HA	3:F:115:VAL:HB	1.84	0.60
1:D:390:THR:HG21	1:D:393:VAL:HG23	1.82	0.60
3:F:20:LEU:CD1	3:F:111:THR:CG2	2.80	0.59
1:D:448:ILE:HD11	1:D:454:LEU:HD22	1.86	0.57
1:D:575:PHE:HA	1:D:578:LEU:HD12	1.87	0.57
3:F:62:PRO:O	3:F:66:ARG:NH1	2.37	0.57
3:F:90:THR:HG23	3:F:114:THR:HA	1.87	0.57
3:C:63:VAL:HG13	3:C:67:PHE:CD2	2.40	0.57
3:F:20:LEU:HB2	3:F:80:LEU:HB3	1.87	0.56
1:A:470:MET:HE3	1:A:482:ILE:HD11	1.85	0.56
1:A:508:PHE:HD2	3:C:50:ILE:HD11	1.70	0.56
1:D:465:THR:CB	6:D:701:ATP:O1B	2.54	0.56
3:C:90:THR:HG23	3:C:114:THR:HA	1.88	0.56
1:A:585:GLU:O	1:A:589:SER:OG	2.22	0.55
1:A:468:LEU:HA	1:A:471:ILE:HD12	1.89	0.55
1:D:401:TRP:CZ2	6:D:701:ATP:C2	2.93	0.55
3:F:20:LEU:HD12	3:F:111:THR:CG2	2.35	0.55
1:A:583:GLU:HG2	1:A:584:LYS:N	2.22	0.55
1:A:610:LEU:HD22	2:B:108:LEU:HD13	1.88	0.55
1:D:468:LEU:HA	1:D:471:ILE:HD12	1.89	0.55
1:D:401:TRP:CE3	1:D:475:LEU:HD13	2.42	0.54
1:D:595:MET:HB3	1:D:600:ARG:HD3	1.88	0.54
1:A:595:MET:HB3	1:A:600:ARG:HD3	1.89	0.53
1:D:400:PHE:HE1	1:D:439:PRO:HD3	1.72	0.53
3:C:22:CYS:HB3	3:C:78:VAL:HG12	1.91	0.53
3:F:20:LEU:HD23	3:F:82:MET:SD	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ASN:HD22	3:C:98:ASN:HD22	1.55	0.52
3:F:18:LEU:HD13	3:F:113:VAL:HG22	1.91	0.52
3:F:66:ARG:NH2	3:F:89:ASP:OD2	2.43	0.52
3:C:2:VAL:CB	3:C:106:SER:HB3	2.39	0.51
1:D:465:THR:OG1	6:D:701:ATP:O1B	2.20	0.51
1:D:508:PHE:O	3:F:58:ARG:CZ	2.58	0.51
2:B:90:THR:HG23	2:B:120:THR:HA	1.91	0.51
3:C:63:VAL:HG22	3:C:67:PHE:CE2	2.45	0.51
3:F:24:ALA:HB3	3:F:76:ASN:HB3	1.92	0.51
1:A:610:LEU:HD22	2:B:108:LEU:CD1	2.40	0.51
1:D:507:ILE:O	1:D:507:ILE:HG22	2.10	0.51
2:E:47:MET:HG2	2:E:48:VAL:N	2.26	0.51
1:D:441:LEU:CD2	1:D:470:MET:HE2	2.29	0.51
2:E:90:THR:HG23	2:E:120:THR:HA	1.92	0.51
1:A:453:LEU:HD23	1:A:613:ALA:HA	1.93	0.51
1:D:453:LEU:HD23	1:D:613:ALA:HA	1.93	0.51
1:A:457:ALA:HB3	1:A:618:ILE:HG12	1.93	0.50
1:A:575:PHE:HA	1:A:578:LEU:HD12	1.93	0.50
3:F:33:ALA:O	3:F:97:LEU:HD12	2.12	0.50
1:A:470:MET:HE3	1:A:482:ILE:CD1	2.42	0.50
3:C:24:ALA:HB3	3:C:76:ASN:HB3	1.94	0.50
2:E:31:ILE:HG12	2:E:99:ILE:HG12	1.93	0.49
2:E:101:GLU:OE2	2:E:112:TYR:OH	2.29	0.49
2:B:7:SER:HB2	2:B:21:ALA:HB3	1.95	0.49
3:F:31:ILE:HG12	3:F:97:LEU:HD11	1.94	0.49
3:F:32:ASN:HD22	3:F:98:ASN:HD22	1.60	0.48
1:D:465:THR:HB	6:D:701:ATP:O1B	2.13	0.48
2:E:7:SER:HB2	2:E:21:ALA:HB3	1.94	0.48
1:D:466:SER:OG	6:D:701:ATP:O1A	2.23	0.48
3:F:18:LEU:HB2	3:F:82:MET:HE3	1.96	0.48
1:A:464:LYS:HE3	6:A:703:ATP:O2B	2.14	0.47
3:C:20:LEU:HB2	3:C:80:LEU:HB3	1.95	0.47
1:D:401:TRP:CE2	6:D:701:ATP:C2	3.02	0.47
1:A:465:THR:HB	6:A:703:ATP:O1B	2.14	0.47
3:F:17:SER:OG	3:F:83:ASN:HA	2.15	0.47
1:D:448:ILE:CD1	1:D:454:LEU:HD22	2.45	0.47
1:A:448:ILE:HD11	1:A:454:LEU:HD13	1.97	0.46
3:F:11:LEU:HD21	3:F:119:ALA:HB2	1.97	0.46
1:D:501:THR:HA	1:D:539:ILE:O	2.16	0.46
2:B:106:PHE:CD1	2:B:106:PHE:N	2.82	0.46
3:C:17:SER:OG	3:C:83:ASN:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:VAL:HG13	2:E:63:VAL:HG11	1.99	0.45
2:E:6:GLU:HB3	2:E:117:THR:HB	1.98	0.45
1:D:390:THR:CG2	1:D:393:VAL:HG23	2.44	0.45
1:D:490:PHE:HD1	1:D:570:LEU:HB2	1.82	0.45
1:D:457:ALA:HB1	2:E:108:LEU:HD21	1.98	0.45
1:D:520:VAL:HG22	1:D:562:VAL:HG23	2.00	0.45
1:A:617:LEU:HD11	1:A:619:LEU:HD11	1.99	0.44
1:A:468:LEU:HD22	1:A:570:LEU:HB3	1.98	0.44
2:B:32:ASN:OD1	2:B:109:THR:HG21	2.17	0.44
3:C:2:VAL:CB	3:C:106:SER:CB	2.95	0.44
1:A:493:GLN:HA	1:A:572:ASP:O	2.18	0.44
1:A:533:PHE:HZ	1:A:548:LEU:HD21	1.83	0.43
1:D:562:VAL:HG12	1:D:595:MET:SD	2.58	0.43
2:E:22:CYS:O	2:E:77:THR:HA	2.18	0.43
1:A:508:PHE:HE2	3:C:50:ILE:HG12	1.81	0.43
1:D:467:LEU:O	1:D:470:MET:HB2	2.19	0.43
2:B:22:CYS:O	2:B:77:THR:HA	2.18	0.43
1:D:460:THR:O	1:D:460:THR:HG22	2.18	0.43
1:A:490:PHE:HD1	1:A:570:LEU:HB2	1.83	0.43
1:A:504:GLU:O	1:A:508:PHE:HB2	2.19	0.43
1:D:513:ASP:HB3	1:D:516:ARG:HB3	2.01	0.43
3:F:20:LEU:HD11	3:F:111:THR:HG23	2.01	0.43
3:F:32:ASN:HB2	3:F:98:ASN:HD22	1.84	0.42
1:A:520:VAL:HG22	1:A:562:VAL:HG23	2.00	0.42
3:F:11:LEU:CD2	3:F:119:ALA:HB2	2.49	0.42
1:D:493:GLN:HA	1:D:572:ASP:O	2.19	0.42
3:F:20:LEU:CD2	3:F:82:MET:SD	3.07	0.42
3:F:69:ILE:HA	3:F:79:TYR:O	2.19	0.42
1:A:470:MET:CE	1:A:482:ILE:CD1	2.92	0.42
1:A:562:VAL:HG12	1:A:595:MET:SD	2.60	0.42
2:B:104:ARG:HA	2:B:105:PRO:HD3	1.75	0.42
2:B:48:VAL:HG13	2:B:63:VAL:HG11	2.01	0.41
1:A:393:VAL:HG13	1:A:394:MET:N	2.35	0.41
1:A:508:PHE:CE2	3:C:50:ILE:HG12	2.55	0.41
3:C:5:GLN:O	3:C:22:CYS:HA	2.19	0.41
3:C:82:MET:HE3	3:C:82:MET:HB2	1.94	0.41
1:D:392:VAL:HG13	1:D:448:ILE:CD1	2.44	0.41
1:D:552:GLN:HA	1:D:555:ARG:NH1	2.36	0.41
1:D:453:LEU:HB2	1:D:600:ARG:NH2	2.36	0.41
3:C:32:ASN:HD22	3:C:98:ASN:ND2	2.18	0.41
3:C:63:VAL:CG1	3:C:67:PHE:CD2	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/229 (90%)	193 (94%)	13 (6%)	0	100	100
1	D	207/229 (90%)	193 (93%)	14 (7%)	0	100	100
2	B	119/149 (80%)	113 (95%)	6 (5%)	0	100	100
2	E	120/149 (80%)	117 (98%)	3 (2%)	0	100	100
3	C	110/143 (77%)	108 (98%)	2 (2%)	0	100	100
3	F	112/143 (78%)	110 (98%)	2 (2%)	0	100	100
All	All	874/1042 (84%)	834 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/197 (82%)	156 (96%)	6 (4%)	34	66
1	D	146/197 (74%)	140 (96%)	6 (4%)	30	63
2	B	92/118 (78%)	89 (97%)	3 (3%)	38	70
2	E	87/118 (74%)	84 (97%)	3 (3%)	37	69
3	C	73/112 (65%)	70 (96%)	3 (4%)	30	63
3	F	81/112 (72%)	77 (95%)	4 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	641/854 (75%)	616 (96%)	25 (4%)	32	64

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	VAL
1	A	466	SER
1	A	467	LEU
1	A	583	GLU
1	A	623	SER
1	A	634	GLN
2	B	61	ASP
2	B	106	PHE
2	B	107	TYR
3	C	31	ILE
3	C	51	SER
3	C	98	ASN
1	D	448	ILE
1	D	547	THR
1	D	573	SER
1	D	583	GLU
1	D	606	LYS
1	D	631	SER
2	E	100	THR
2	E	103	SER
2	E	122	SER
3	F	31	ILE
3	F	52	SER
3	F	114	THR
3	F	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3	GLN
2	B	33	ASN
3	C	1	GLN
3	C	73	ASN
3	C	76	ASN
3	C	83	ASN
3	C	98	ASN

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Mol	Chain	Res	Type
3	F	83	ASN
3	F	98	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ATP	A	703	5	26,33,33	1.17	2 (7%)	31,52,52	1.55	7 (22%)
6	ATP	D	701	-	26,33,33	1.09	1 (3%)	31,52,52	1.55	6 (19%)
4	GOL	A	701	-	5,5,5	0.11	0	5,5,5	0.26	0

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	ATP	A	703	5	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	D	701	-	-	3/18/38/38	0/3/3/3
4	GOL	A	701	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	ATP	C2'-C1'	-2.55	1.49	1.53
6	A	703	ATP	C5-C4	2.39	1.47	1.40
6	D	701	ATP	C5-C4	2.35	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	703	ATP	N3-C2-N1	-3.45	123.29	128.68
6	D	701	ATP	PB-O3B-PG	-3.34	121.37	132.83
6	A	703	ATP	C3'-C2'-C1'	3.03	105.54	100.98
6	A	703	ATP	C4-C5-N7	-2.97	106.31	109.40
6	D	701	ATP	PA-O3A-PB	-2.72	123.50	132.83
6	D	701	ATP	O3'-C3'-C4'	-2.70	103.25	111.05
6	D	701	ATP	N3-C2-N1	-2.63	124.57	128.68
6	D	701	ATP	O4'-C1'-C2'	-2.47	103.31	106.93
6	D	701	ATP	O3G-PG-O2G	2.29	116.40	107.64
6	A	703	ATP	C2-N1-C6	2.20	122.52	118.75
6	A	703	ATP	C5'-C4'-C3'	-2.03	107.59	115.18
6	A	703	ATP	PA-O3A-PB	-2.03	125.88	132.83
6	A	703	ATP	C2'-C3'-C4'	2.00	106.53	102.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	GOL	O1-C1-C2-C3
6	A	703	ATP	PB-O3B-PG-O3G
4	A	701	GOL	O1-C1-C2-O2
6	D	701	ATP	O4'-C4'-C5'-O5'
4	A	701	GOL	C1-C2-C3-O3
6	D	701	ATP	C3'-C4'-C5'-O5'
4	A	701	GOL	O2-C2-C3-O3
6	A	703	ATP	C5'-O5'-PA-O1A
6	D	701	ATP	C5'-O5'-PA-O1A

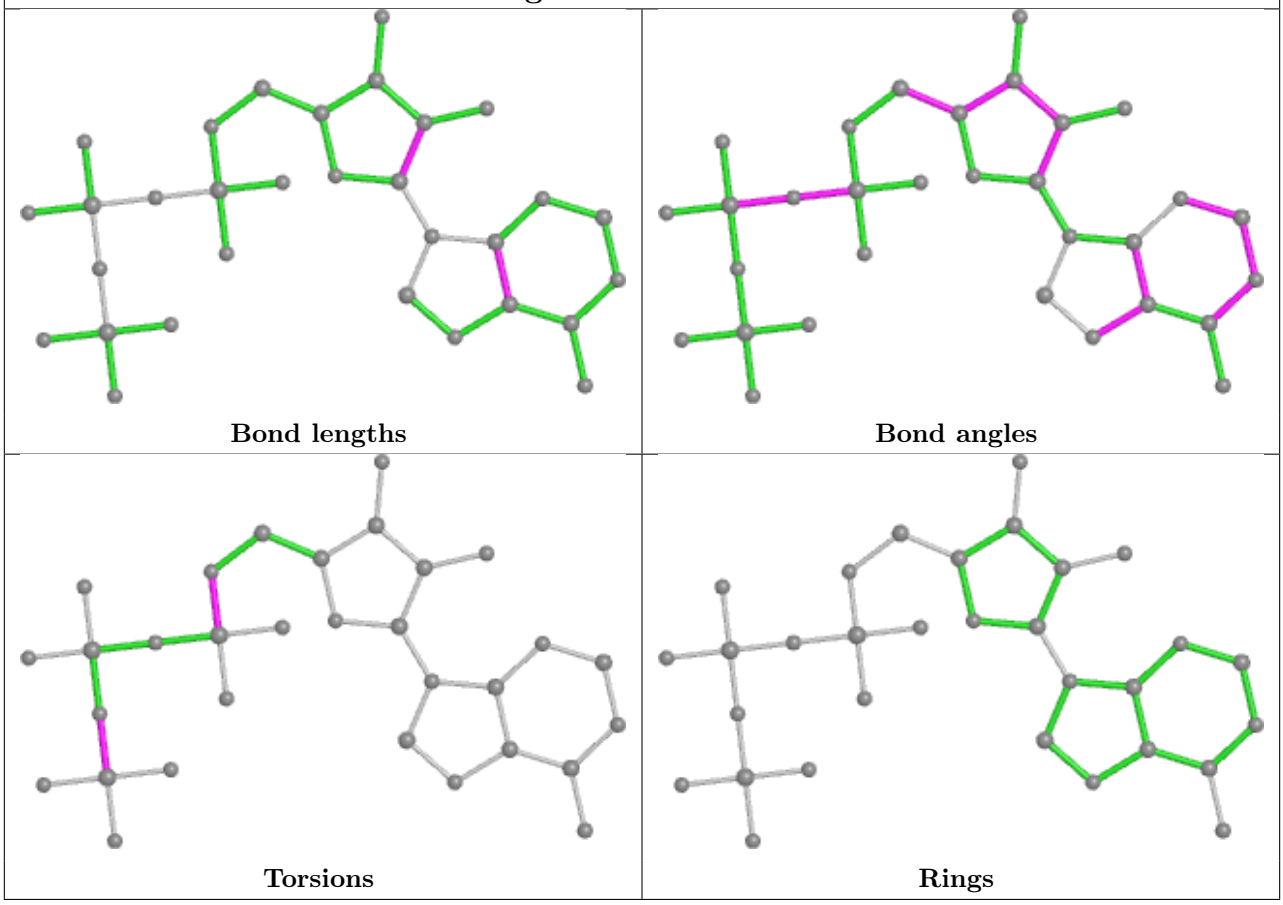
There are no ring outliers.

2 monomers are involved in 11 short contacts:

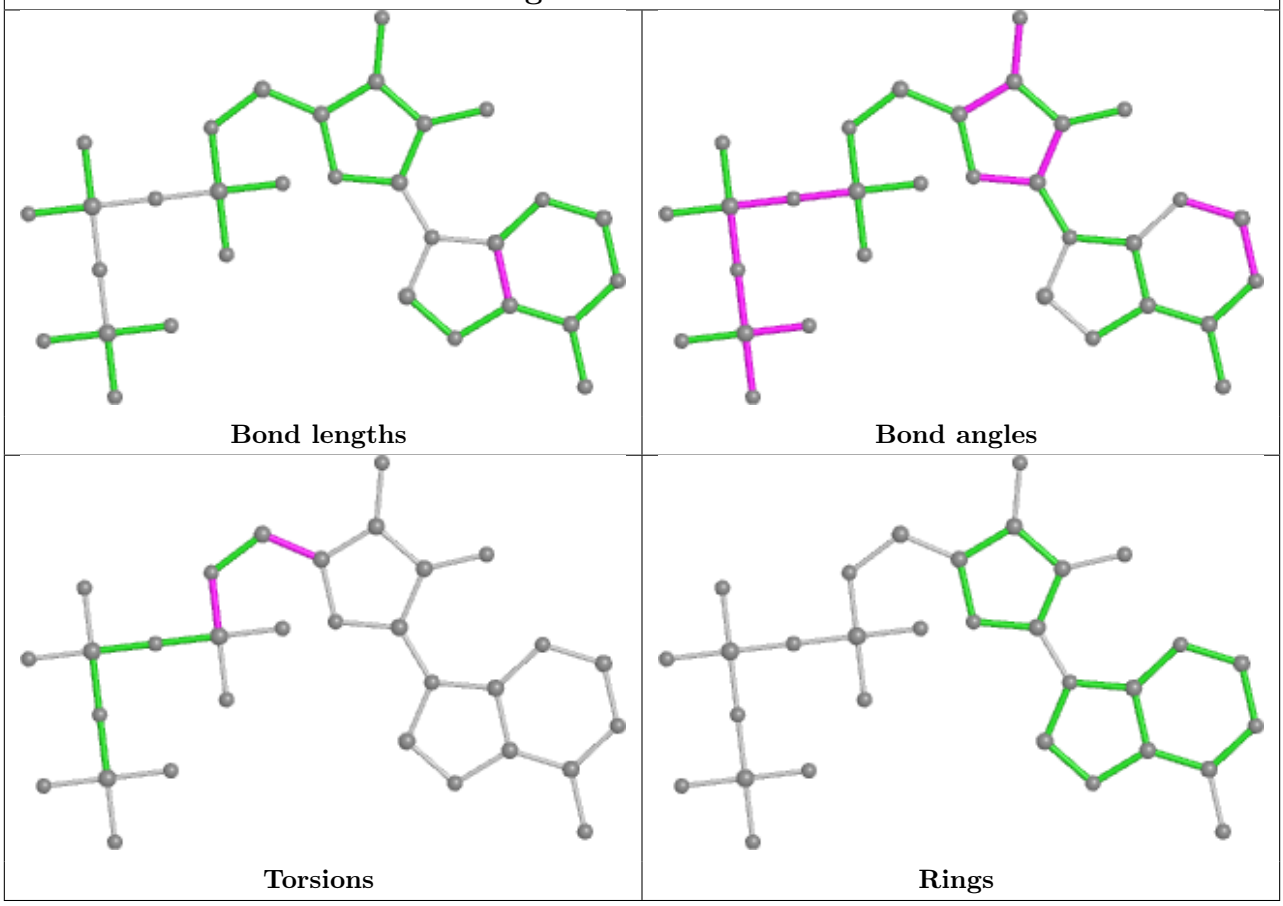
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	ATP	5	0
6	D	701	ATP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 703



Ligand ATP D 701



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	210/229 (91%)	0.41	12 (5%)	23	20	28, 53, 89, 116	0
1	D	211/229 (92%)	0.40	11 (5%)	27	24	22, 49, 92, 106	0
2	B	121/149 (81%)	0.33	3 (2%)	57	56	19, 47, 76, 96	0
2	E	122/149 (81%)	0.21	3 (2%)	57	56	22, 43, 69, 93	0
3	C	114/143 (79%)	0.46	9 (7%)	12	10	31, 59, 81, 116	0
3	F	116/143 (81%)	0.08	0	100	100	25, 45, 69, 92	0
All	All	894/1042 (85%)	0.33	38 (4%)	35	32	19, 50, 85, 116	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	THR	5.9
3	C	75	GLN	4.9
1	A	475	LEU	4.5
3	C	116	SER	4.3
1	D	478	SER	3.8
2	E	109	THR	3.5
2	B	42	GLY	3.3
1	A	485	SER	3.2
3	C	74	ALA	3.2
1	D	627	TYR	3.1
1	A	544	GLY	3.0
1	A	481	LYS	3.0
1	A	603	VAL	2.9
1	D	398	THR	2.9
2	E	24	ALA	2.9
2	E	108	LEU	2.9
1	A	486	GLY	2.8
1	A	530	ILE	2.7
3	C	41	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	481	LYS	2.7
3	C	24	ALA	2.7
3	C	76	ASN	2.7
3	C	53	SER	2.6
1	D	401	TRP	2.6
1	A	478	SER	2.6
1	A	399	ALA	2.5
3	C	57	THR	2.4
1	D	485	SER	2.3
3	C	92	VAL	2.2
2	B	28	ILE	2.1
1	A	398	THR	2.1
1	D	400	PHE	2.1
1	A	394	MET	2.1
1	D	630	PHE	2.1
1	D	475	LEU	2.0
2	B	12	VAL	2.0
1	A	482	ILE	2.0
1	D	397	VAL	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
6	ATP	D	701	31/31	0.84	0.19	81,88,91,91	0
6	ATP	A	703	31/31	0.90	0.17	61,73,88,89	0
4	GOL	A	701	6/6	0.90	0.17	44,47,49,50	0
5	MG	D	702	1/1	0.93	0.14	34,34,34,34	0

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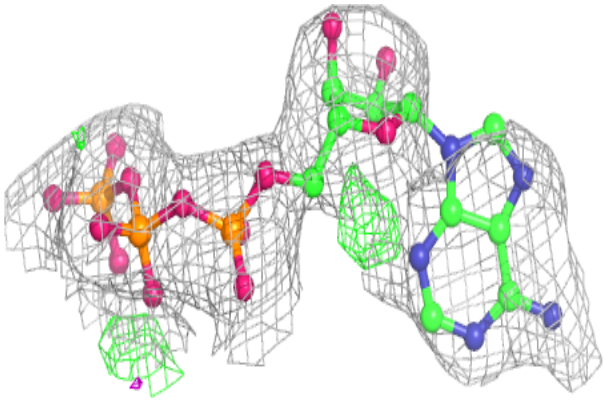
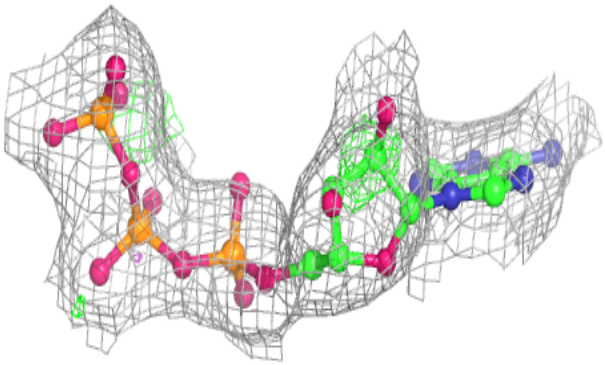
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	702	1/1	0.97	0.10	56,56,56,56	0

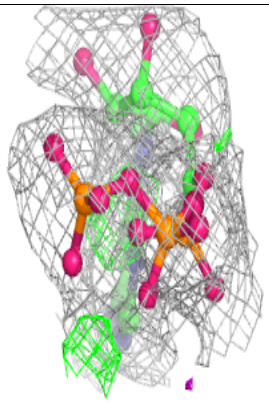
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP D 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

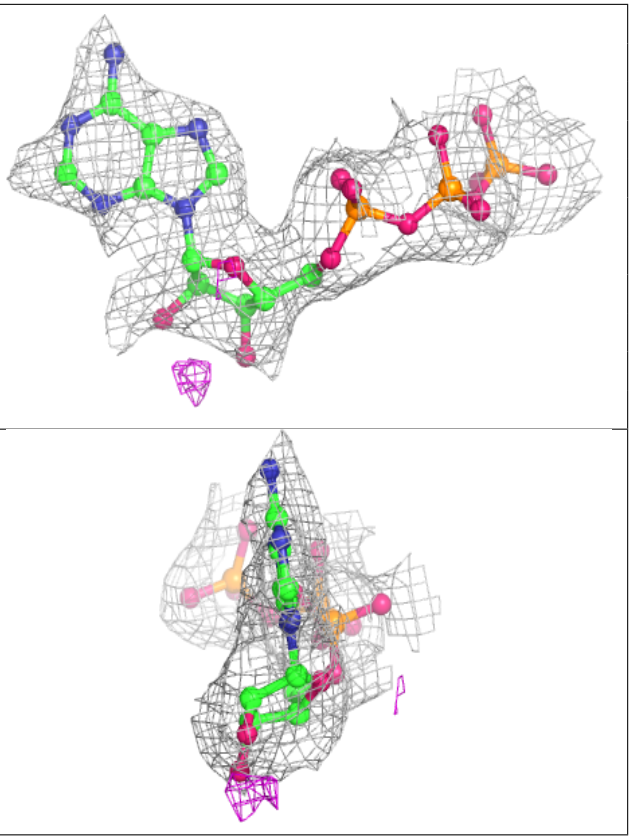






Electron density around ATP A 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.