



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:45 AM UTC

PDB ID : 5FL7 / pdb_00005fl7
Title : Structure of the F1c10 complex from Yarrowia lipolytica ATP synthase
Authors : Parey, K.; Bublitz, M.; Meier, T.
Deposited on : 2015-10-22
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

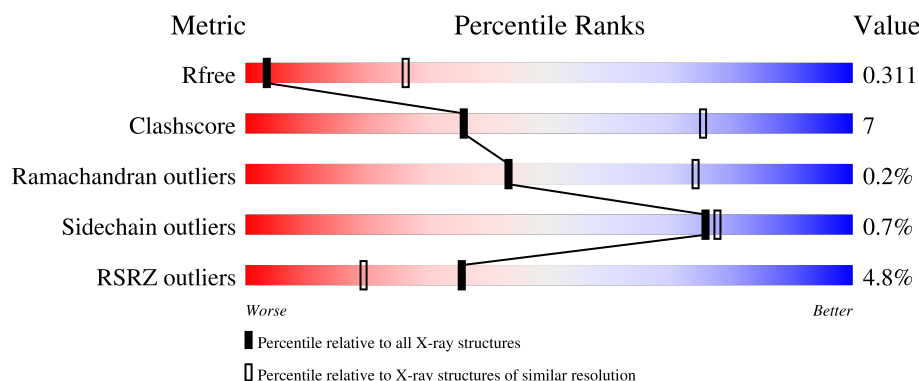
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. 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	536	
1	B	536	
1	C	536	
2	D	509	
2	E	509	

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Mol	Chain	Length	Quality of chain
2	F	509	
3	G	293	
4	H	137	
5	I	16	
6	K	76	
6	L	76	
6	M	76	
6	N	76	
6	O	76	
6	P	76	
6	Q	76	
6	R	76	
6	S	76	
6	T	76	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 30119 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 ATP SYNTHASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3699	2341	645	704	9			
1	B	479	Total	C	N	O	S	0	0	0
			3653	2310	638	696	9			
1	C	485	Total	C	N	O	S	0	0	0
			3699	2341	645	704	9			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3535	2226	605	696	8			
2	E	468	Total	C	N	O	S	0	0	0
			3524	2219	603	694	8			
2	F	470	Total	C	N	O	S	0	0	0
			3535	2226	605	696	8			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA CHAIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	267	Total	C	N	O	S	0	0	0
			2068	1291	357	411	9			

- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	113	Total	C	N	O	0	0	0
			843	525	135	183			

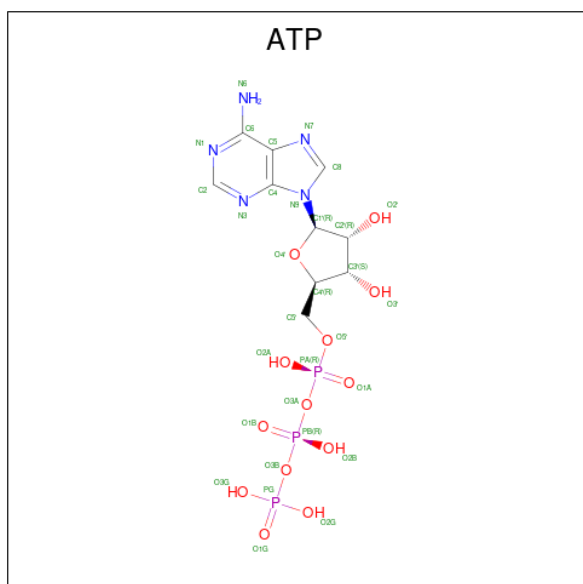
- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	73	Total	C	N	O	S	0	0	0
			524	353	82	88	1			
6	L	72	Total	C	N	O	S	0	0	0
			512	344	81	86	1			
6	M	75	Total	C	N	O	S	0	0	0
			536	361	84	90	1			
6	N	75	Total	C	N	O	S	0	0	0
			537	361	84	90	2			
6	O	75	Total	C	N	O	S	0	0	0
			537	361	84	91	1			
6	P	75	Total	C	N	O	S	0	0	0
			537	361	84	90	2			
6	Q	76	Total	C	N	O	S	0	0	0
			544	366	85	91	2			
6	R	74	Total	C	N	O	S	0	0	0
			529	356	83	89	1			
6	S	74	Total	C	N	O	S	0	0	0
			529	356	83	89	1			
6	T	74	Total	C	N	O	S	0	0	0
			529	356	83	89	1			

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

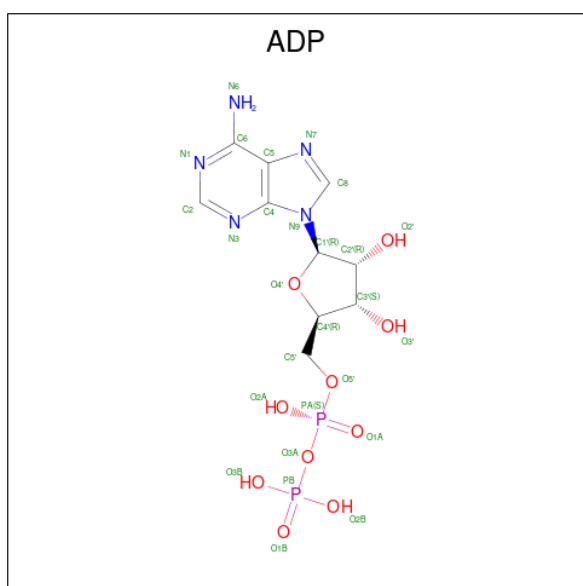


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

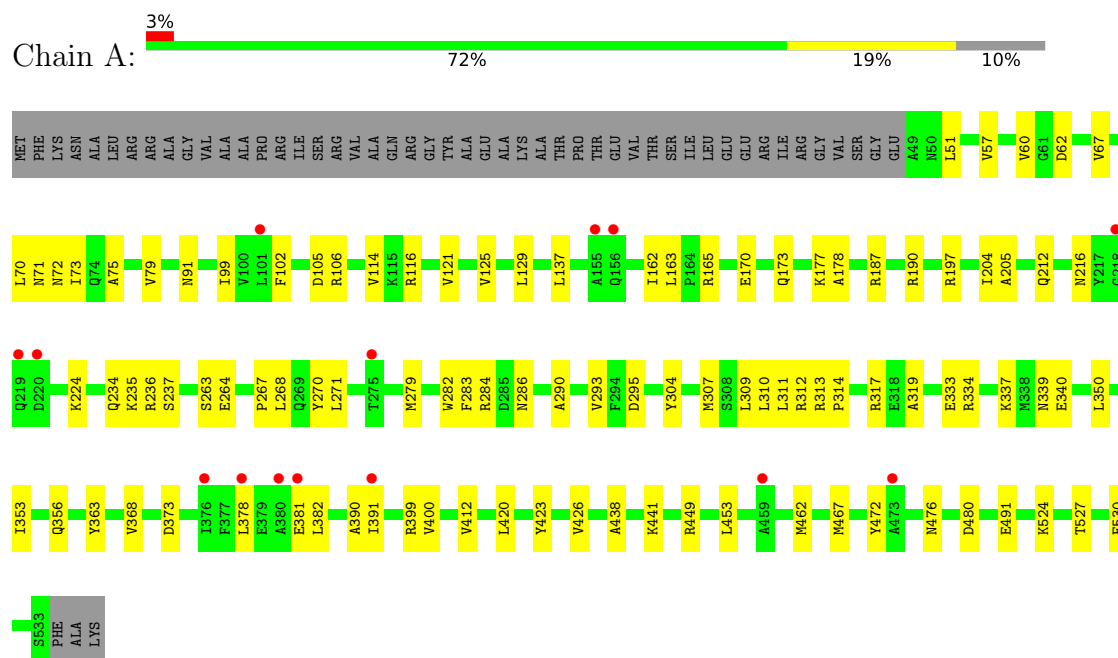
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total 3	O 3	0	0
10	B	3	Total 3	O 3	0	0
10	C	3	Total 3	O 3	0	0
10	D	4	Total 4	O 4	0	0
10	F	4	Total 4	O 4	0	0

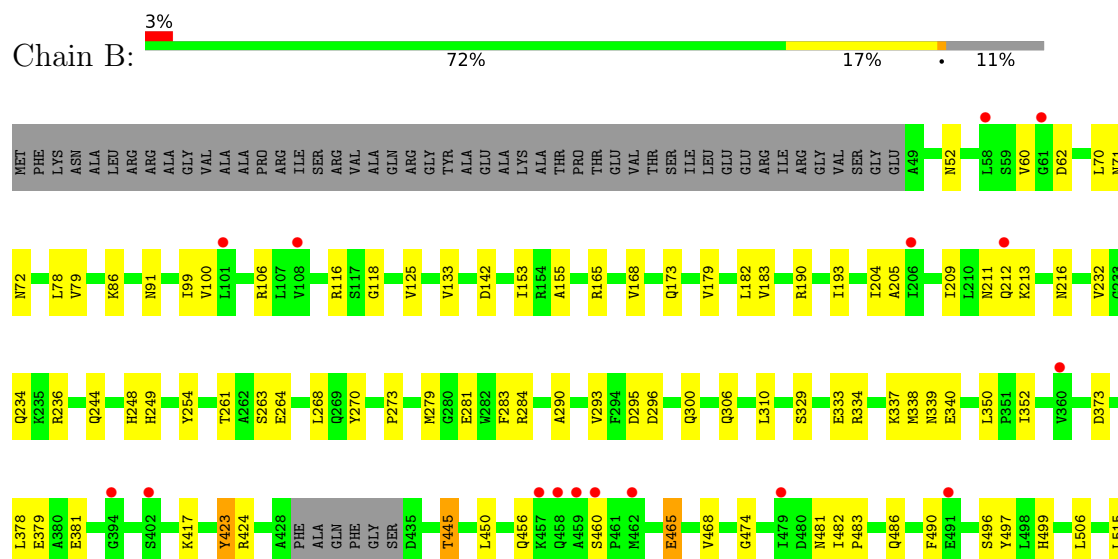
3 Residue-property plots

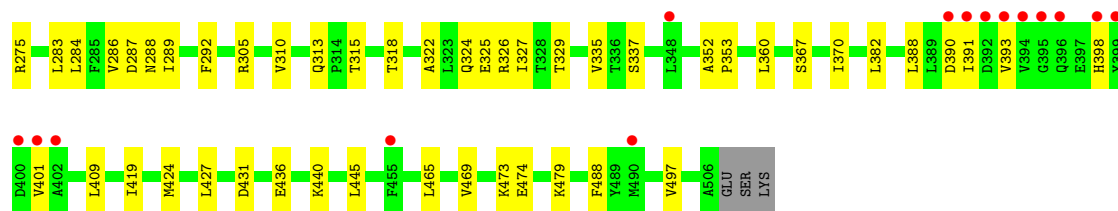
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP SYNTHASE SUBUNIT ALPHA

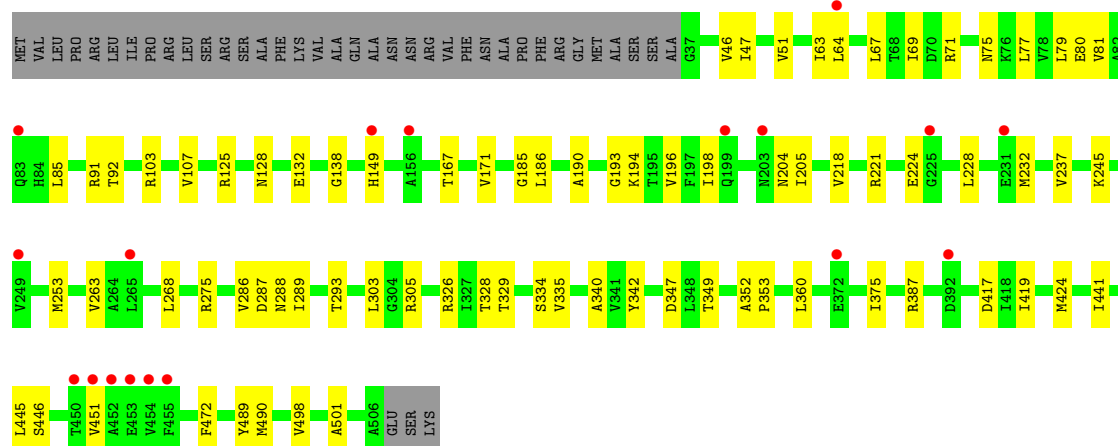


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA

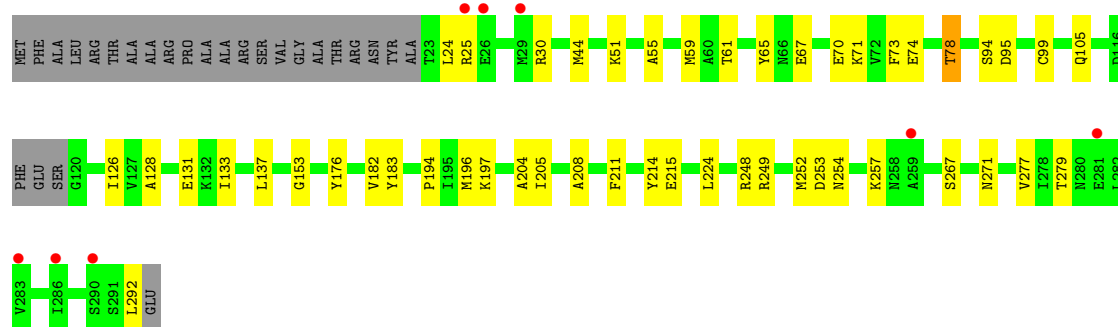
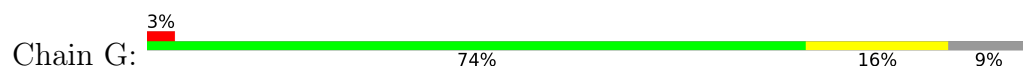




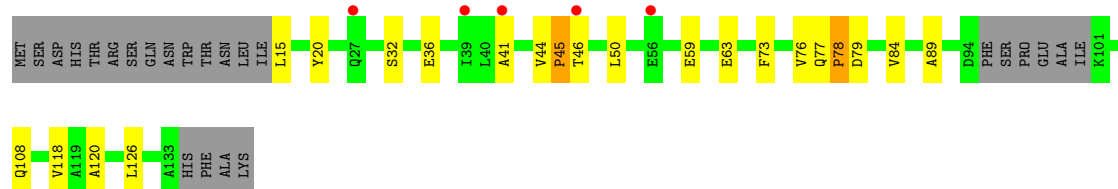
• Molecule 2: ATP SYNTHASE SUBUNIT BETA



• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA CHAIN, MITOCHONDRIAL



• Molecule 4: ATP SYNTHASE DELTA CHAIN, MITOCHONDRIAL



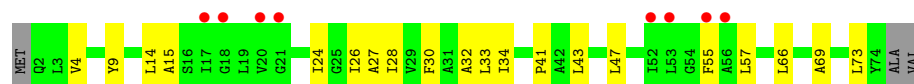
- Molecule 5: ATP SYNTHASE EPSILON CHAIN, MITOCHONDRIAL

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain K:  11% 70% 26%



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain L:  9% 76% 18% 5%



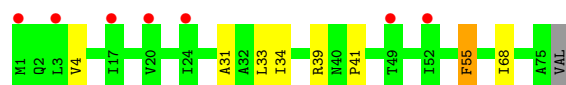
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain M:  8% 76% 22%



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain N:  9% 88% 9% ..



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain O:  4% 83% 14% ..

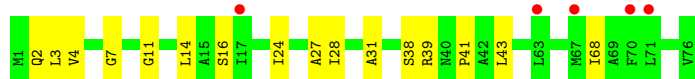
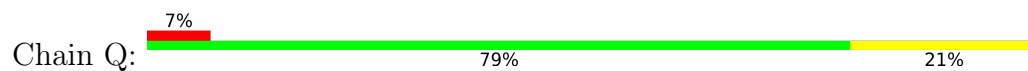


- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

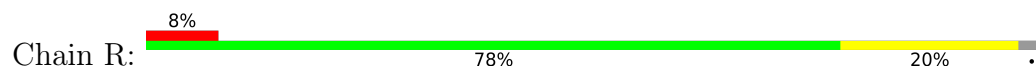
Chain P:  5% 80% 18%



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



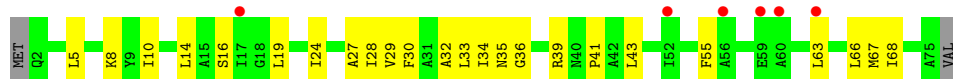
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.50Å 182.20Å 193.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 3.50 49.37 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.37-3.50) 99.9 (49.37-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.274 , 0.305 0.278 , 0.311	Depositor DCC
R_{free} test set	1898 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	157.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 98.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	30119	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, 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	0.08	0/3755	0.27	0/5076
1	B	0.09	0/3706	0.26	0/5009
1	C	0.09	0/3755	0.29	0/5076
2	D	0.09	0/3587	0.27	0/4868
2	E	0.09	0/3576	0.27	0/4853
2	F	0.09	0/3587	0.28	0/4868
3	G	0.08	0/2090	0.28	0/2812
4	H	0.11	0/851	0.31	0/1157
6	K	0.08	0/532	0.24	0/720
6	L	0.06	0/519	0.21	0/702
6	M	0.07	0/544	0.21	0/737
6	N	0.06	0/545	0.19	0/737
6	O	0.10	0/545	0.29	0/737
6	P	0.06	0/545	0.19	0/737
6	Q	0.09	0/552	0.27	0/747
6	R	0.07	0/537	0.21	0/727
6	S	0.07	0/537	0.21	0/727
6	T	0.08	0/537	0.24	0/727
All	All	0.09	0/30300	0.27	0/41017

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3699	0	3781	63	0
1	B	3653	0	3741	53	0
1	C	3699	0	3781	52	0
2	D	3535	0	3562	63	0
2	E	3524	0	3551	58	0
2	F	3535	0	3562	50	0
3	G	2068	0	2099	32	0
4	H	843	0	824	18	0
5	I	80	0	18	0	0
6	K	524	0	565	20	0
6	L	512	0	556	15	0
6	M	536	0	579	15	0
6	N	537	0	582	8	0
6	O	537	0	579	10	0
6	P	537	0	582	15	0
6	Q	544	0	591	15	0
6	R	529	0	570	15	0
6	S	529	0	570	22	0
6	T	529	0	570	22	0
7	A	31	0	12	0	0
7	B	31	0	12	0	0
7	C	31	0	12	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	D	27	0	12	3	0
9	F	27	0	12	3	0
10	A	3	0	0	0	0
10	B	3	0	0	0	0
10	C	3	0	0	0	0
10	D	4	0	0	0	0
10	F	4	0	0	2	0
All	All	30119	0	30723	443	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 7.

All (443) 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:B:329:SER:HB2	2:F:253:MET:HB3	1.66	0.77
3:G:208:ALA:HB3	3:G:211:PHE:HB2	1.71	0.73
2:D:189:GLY:O	2:D:194:LYS:NZ	2.22	0.73
1:C:370:SER:HB3	2:D:291:ARG:HH22	1.57	0.70
1:B:450:LEU:HD21	1:B:474:GLY:HA3	1.73	0.70
1:C:309:LEU:HD21	1:C:315:PRO:HB3	1.76	0.67
2:D:183:LYS:HZ1	2:D:324:GLN:HB3	1.60	0.67
1:A:236:ARG:NH1	2:D:153:PRO:O	2.28	0.66
2:F:198:ILE:HD11	2:F:340:ALA:HB2	1.76	0.66
6:L:3:LEU:HD21	6:M:3:LEU:HD13	1.77	0.66
6:R:68:ILE:HD12	6:S:16:SER:HB3	1.77	0.66
1:A:129:LEU:HD13	1:A:279:MET:HE3	1.77	0.66
2:D:375:ILE:HG23	2:D:446:SER:HB2	1.78	0.65
1:A:177:LYS:NZ	1:A:491:GLU:OE2	2.30	0.65
6:P:4:VAL:HG23	6:Q:2:GLN:HG3	1.79	0.65
1:B:106:ARG:HA	2:E:63:ILE:HB	1.77	0.65
1:A:121:VAL:HG11	1:A:271:LEU:HD21	1.78	0.65
3:G:126:ILE:HD13	3:G:137:LEU:HD23	1.78	0.65
2:E:69:ILE:HG12	2:E:107:VAL:HG22	1.79	0.65
3:G:267:SER:O	3:G:271:ASN:ND2	2.30	0.65
6:S:26:ILE:HD11	6:S:59:GLU:HB2	1.79	0.64
6:K:47:LEU:HD22	6:L:34:ILE:HG23	1.80	0.64
1:B:62:ASP:OD1	2:E:305:ARG:NH2	2.30	0.64
3:G:128:ALA:HB1	3:G:133:ILE:HG23	1.80	0.64
6:L:47:LEU:HD13	6:M:34:ILE:HG23	1.79	0.63
1:A:106:ARG:NH1	2:D:65:ASN:OD1	2.31	0.63
2:D:500:LYS:HE2	2:D:504:LEU:HD11	1.79	0.63
2:F:417:ASP:OD2	3:G:30:ARG:NH2	2.31	0.63
1:C:235:LYS:NZ	1:C:237:SER:OG	2.29	0.62
2:D:198:ILE:HD11	2:D:340:ALA:HB2	1.81	0.62
1:B:70:LEU:O	2:F:103:ARG:NH2	2.33	0.62
1:A:235:LYS:HE3	1:A:237:SER:HB3	1.81	0.62
2:D:347:ASP:HB2	3:G:25:ARG:HH12	1.64	0.62
1:B:456:GLN:NE2	1:B:460:SER:O	2.33	0.62
6:S:26:ILE:HG23	6:S:55:PHE:HB2	1.81	0.62
6:M:43:LEU:HD11	6:N:41:PRO:HB3	1.81	0.61
2:E:67:LEU:HB2	2:E:79:LEU:HB2	1.83	0.61
1:A:197:ARG:NH1	1:A:356:GLN:OE1	2.34	0.61
2:D:408:THR:HG23	2:D:434:THR:HG23	1.81	0.61
2:D:461:ARG:NH1	2:D:496:GLU:OE2	2.34	0.61
2:F:71:ARG:HH21	2:F:77:LEU:HD22	1.65	0.61
1:A:62:ASP:OD1	2:D:305:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLN:HG3	1:C:225:LEU:HD22	1.83	0.60
2:E:275:ARG:HD3	2:E:335:VAL:HG23	1.83	0.60
6:R:43:LEU:HD11	6:S:41:PRO:HG3	1.82	0.60
6:P:43:LEU:HD11	6:Q:41:PRO:HG3	1.82	0.60
6:Q:43:LEU:HD11	6:R:41:PRO:HG3	1.82	0.60
6:R:33:LEU:HA	6:S:34:ILE:HG21	1.83	0.60
1:A:235:LYS:NZ	2:D:361:ASP:OD1	2.35	0.59
6:S:68:ILE:HD11	6:T:66:LEU:HD12	1.85	0.59
1:C:121:VAL:HG11	1:C:271:LEU:HD21	1.84	0.59
2:E:419:ILE:HD12	2:E:424:MET:HG2	1.84	0.59
6:K:41:PRO:HG3	6:T:43:LEU:HD11	1.85	0.58
1:C:90:LEU:HD11	1:C:307:MET:HE2	1.85	0.58
2:D:41:GLY:O	2:D:107:VAL:N	2.35	0.58
1:C:234:GLN:NE2	1:C:295:ASP:OD2	2.37	0.58
1:B:212:GLN:O	1:B:216:ASN:ND2	2.36	0.58
1:C:125:VAL:HG12	1:C:279:MET:HA	1.86	0.58
2:F:194:LYS:HB2	10:F:2001:HOH:O	2.04	0.58
1:A:70:LEU:HD13	1:A:73:ILE:HD12	1.86	0.57
2:D:268:LEU:HD13	2:D:327:ILE:HG12	1.86	0.57
1:C:339:ASN:OD1	1:C:340:GLU:N	2.37	0.57
6:M:28:ILE:HG22	6:N:31:ALA:HB2	1.87	0.57
2:F:125:ARG:NH2	2:F:138:GLY:O	2.37	0.57
1:A:234:GLN:NE2	1:A:295:ASP:OD2	2.38	0.57
1:A:173:GLN:O	1:A:212:GLN:NE2	2.37	0.56
2:D:418:ILE:HG23	2:D:422:LEU:HD12	1.86	0.56
2:E:388:LEU:HD22	2:E:393:VAL:HG11	1.85	0.56
6:K:28:ILE:HB	6:L:27:ALA:HB1	1.86	0.56
2:F:167:THR:O	2:F:204:ASN:ND2	2.39	0.56
6:K:30:PHE:CZ	6:T:29:VAL:HG22	2.40	0.56
1:C:57:VAL:HG22	1:C:67:VAL:HG22	1.88	0.56
1:B:284:ARG:NH1	1:B:338:MET:SD	2.79	0.56
1:C:177:LYS:HD2	1:C:454:LEU:HA	1.88	0.56
1:A:282:TRP:O	1:A:286:ASN:ND2	2.35	0.56
1:C:192:LEU:HB2	1:C:372:THR:HG21	1.88	0.56
6:L:5:LEU:HA	6:L:8:LYS:HD3	1.88	0.56
1:A:263:SER:HB3	2:D:325:GLU:HG3	1.88	0.56
2:D:69:ILE:HG12	2:D:107:VAL:HG22	1.88	0.56
2:F:275:ARG:NH1	2:F:328:THR:O	2.39	0.56
1:A:178:ALA:HB3	1:A:391:ILE:HD12	1.87	0.55
1:B:236:ARG:HG2	1:B:261:THR:HG21	1.88	0.55
2:D:433:LEU:HD21	2:D:437:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:ILE:HG13	2:E:283:LEU:HD11	1.89	0.55
3:G:24:LEU:HD22	3:G:277:VAL:HG21	1.89	0.55
3:G:95:ASP:HB3	3:G:131:GLU:H	1.71	0.55
1:B:339:ASN:OD1	1:B:340:GLU:N	2.39	0.55
6:O:43:LEU:HD21	6:P:41:PRO:HB3	1.88	0.55
6:K:43:LEU:HD11	6:L:41:PRO:HG3	1.87	0.55
1:A:304:TYR:HA	1:A:307:MET:HE3	1.88	0.55
2:E:401:VAL:HG11	2:E:469:VAL:HG13	1.88	0.54
1:B:78:LEU:HD11	1:B:86:LYS:HB3	1.88	0.54
1:B:293:VAL:HG22	1:B:350:LEU:HB2	1.89	0.54
1:B:62:ASP:HB3	1:B:310:LEU:HD22	1.88	0.54
3:G:249:ARG:O	3:G:253:ASP:N	2.36	0.54
1:A:339:ASN:OD1	1:A:340:GLU:N	2.40	0.54
1:C:133:VAL:HB	1:C:142:ASP:HB3	1.89	0.54
4:H:36:GLU:OE1	6:P:40:ASN:ND2	2.35	0.54
2:D:167:THR:HA	2:D:205:ILE:HD11	1.90	0.54
2:F:80:GLU:OE2	2:F:149:HIS:NE2	2.40	0.54
1:B:179:VAL:HG13	1:B:183:VAL:HG23	1.90	0.54
2:E:63:ILE:HG22	2:E:64:LEU:HG	1.90	0.54
4:H:44:VAL:O	4:H:46:THR:N	2.39	0.54
1:A:399:ARG:HH12	2:E:190:ALA:HB3	1.73	0.54
1:A:62:ASP:HB3	1:A:310:LEU:HD13	1.90	0.53
1:B:486:GLN:O	1:B:490:PHE:N	2.41	0.53
6:S:68:ILE:HD12	6:T:16:SER:HB3	1.89	0.53
1:A:309:LEU:HD11	1:A:319:ALA:HB1	1.90	0.53
2:E:81:VAL:HA	2:E:92:THR:HG22	1.90	0.53
2:F:193:GLY:HA2	9:F:600:ADP:O1A	2.08	0.53
6:K:66:LEU:HD12	6:T:68:ILE:HD11	1.89	0.53
1:A:293:VAL:HG22	1:A:350:LEU:HB2	1.89	0.53
2:F:194:LYS:N	9:F:600:ADP:O1B	2.40	0.53
4:H:77:GLN:O	4:H:79:ASP:N	2.35	0.53
1:A:91:ASN:HB2	2:E:47:ILE:HG12	1.90	0.53
1:C:159:ALA:HB3	2:D:254:ASN:HD22	1.72	0.53
1:C:93:GLU:O	2:D:103:ARG:NH1	2.40	0.53
1:A:170:GLU:OE2	1:A:337:LYS:NZ	2.42	0.53
1:A:412:VAL:HG12	1:A:472:TYR:HD1	1.74	0.53
1:C:284:ARG:NH1	1:C:334:ARG:O	2.41	0.53
1:A:527:THR:HA	1:A:530:PHE:CE2	2.44	0.53
2:D:448:PRO:HD3	2:D:490:MET:HA	1.91	0.53
2:F:375:ILE:HG23	2:F:446:SER:HB2	1.89	0.53
1:B:244:GLN:O	1:B:248:HIS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ILE:HD12	1:B:378:LEU:HD11	1.90	0.52
2:D:183:LYS:HZ1	2:D:359:HIS:HB3	1.75	0.52
3:G:70:GLU:O	3:G:74:GLU:N	2.41	0.52
6:O:3:LEU:HB3	6:P:2:GLN:HG2	1.90	0.52
2:F:171:VAL:HG12	2:F:445:LEU:HD22	1.92	0.52
6:L:43:LEU:HD11	6:M:41:PRO:HG3	1.91	0.52
1:C:456:GLN:NE2	1:C:460:SER:O	2.31	0.52
2:F:85:LEU:HD21	2:F:91:ARG:HE	1.75	0.52
2:D:300:SER:HB2	2:D:305:ARG:HD2	1.90	0.52
2:E:60:LEU:HD21	2:E:88:ASN:HA	1.91	0.52
6:S:61:THR:HB	6:T:19:LEU:HD21	1.91	0.52
6:S:43:LEU:HD11	6:T:41:PRO:HG3	1.90	0.52
1:B:445:THR:HG23	1:B:481:ASN:HB2	1.91	0.52
1:C:509:ILE:HG23	1:C:513:GLY:HA2	1.91	0.52
6:N:4:VAL:HG23	6:O:2:GLN:HG3	1.91	0.52
2:F:128:ASN:HD21	2:F:132:GLU:HB3	1.74	0.52
6:S:11:GLY:HA2	6:S:14:LEU:HB2	1.91	0.52
1:B:496:SER:O	1:B:499:HIS:ND1	2.36	0.51
1:C:204:ILE:HD12	1:C:378:LEU:HD11	1.91	0.51
3:G:214:TYR:HA	4:H:45:PRO:HB2	1.92	0.51
4:H:108:GLN:HA	4:H:126:LEU:HD21	1.90	0.51
6:S:14:LEU:HD13	6:T:14:LEU:HG	1.91	0.51
6:Q:4:VAL:HG13	6:R:9:TYR:HE2	1.76	0.51
1:B:205:ALA:HB1	1:B:293:VAL:HG11	1.91	0.51
6:R:21:GLY:HA2	6:S:24:ILE:HG13	1.91	0.51
1:A:312:ARG:HH12	3:G:292:LEU:HD12	1.76	0.51
2:E:174:LEU:HA	2:E:398:HIS:HE1	1.74	0.51
2:F:489:TYR:CD1	2:F:490:MET:HG2	2.46	0.51
3:G:182:VAL:HG22	3:G:196:MET:HG2	1.92	0.51
4:H:59:GLU:HB2	4:H:63:GLU:HB2	1.91	0.51
6:K:14:LEU:HD21	6:T:14:LEU:HD13	1.92	0.51
3:G:99:CYS:HA	3:G:248:ARG:HA	1.92	0.51
1:A:79:VAL:HG21	1:A:99:ILE:HD13	1.93	0.51
1:C:79:VAL:HG21	1:C:99:ILE:HD13	1.92	0.51
3:G:105:GLN:HE21	3:G:194:PRO:HG3	1.75	0.51
1:A:284:ARG:NH1	1:A:334:ARG:O	2.44	0.51
3:G:55:ALA:O	3:G:59:MET:N	2.44	0.51
4:H:45:PRO:HA	4:H:76:VAL:HB	1.92	0.51
2:E:268:LEU:HD21	2:E:326:ARG:HB2	1.93	0.50
2:F:347:ASP:OD1	2:F:349:THR:OG1	2.26	0.50
1:A:105:ASP:HB3	2:D:63:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:GLN:O	1:C:211:ASN:ND2	2.44	0.50
2:E:367:SER:HB3	2:E:370:ILE:HG12	1.94	0.50
6:K:9:TYR:CD2	6:T:8:LYS:HG2	2.47	0.50
1:C:281:GLU:OE2	1:C:284:ARG:NH2	2.44	0.50
2:F:268:LEU:HD21	2:F:326:ARG:HB2	1.93	0.50
4:H:41:ALA:HB3	6:O:42:ALA:HB2	1.94	0.50
1:A:381:GLU:OE2	2:D:410:GLN:NE2	2.44	0.50
1:C:284:ARG:HG2	1:C:338:MET:HE2	1.92	0.50
1:A:472:TYR:O	1:A:476:ASN:ND2	2.37	0.50
1:C:215:TRP:CD1	1:C:223:LYS:HB3	2.47	0.50
2:D:286:VAL:HG11	2:D:289:ILE:HD13	1.94	0.50
1:A:317:ARG:HH11	1:A:363:TYR:HB2	1.77	0.50
1:C:241:GLN:HE22	2:F:387:ARG:HE	1.60	0.50
1:B:190:ARG:O	1:B:373:ASP:N	2.45	0.50
1:B:263:SER:HB3	2:E:325:GLU:HG3	1.94	0.50
3:G:254:ASN:HA	3:G:257:LYS:HG2	1.93	0.50
1:A:67:VAL:HG21	1:A:114:VAL:HG21	1.94	0.49
1:A:204:ILE:HD12	1:A:378:LEU:HD11	1.92	0.49
1:B:283:PHE:HB2	1:B:290:ALA:HB2	1.94	0.49
6:K:30:PHE:HA	6:K:33:LEU:HB3	1.94	0.49
1:B:72:ASN:O	1:B:116:ARG:NH1	2.45	0.49
1:C:201:LYS:N	7:C:600:ATP:O1B	2.39	0.49
4:H:20:TYR:OH	4:H:84:VAL:O	2.24	0.49
6:T:32:ALA:O	6:T:36:GLY:N	2.46	0.49
1:A:283:PHE:HB2	1:A:290:ALA:HB2	1.94	0.49
2:E:67:LEU:HD12	2:E:92:THR:HG21	1.94	0.49
6:K:73:LEU:HD11	6:T:68:ILE:HG23	1.93	0.49
6:Q:28:ILE:HG22	6:R:31:ALA:HB2	1.95	0.49
1:A:75:ALA:HB3	2:E:100:GLY:H	1.78	0.49
1:C:150:GLU:HG2	1:C:151:PHE:CD2	2.47	0.49
2:D:194:LYS:NZ	9:D:600:ADP:O2B	2.33	0.49
2:D:412:TYR:HE1	2:D:435:VAL:HG13	1.77	0.49
1:C:198:GLN:HA	7:C:600:ATP:O3B	2.12	0.49
2:F:190:ALA:HB2	2:F:342:TYR:HE1	1.78	0.49
1:B:165:ARG:NH2	1:B:333:GLU:O	2.45	0.49
2:F:69:ILE:HG12	2:F:107:VAL:HG22	1.93	0.49
2:D:67:LEU:HB2	2:D:79:LEU:HB2	1.94	0.49
2:E:163:GLU:OE2	2:E:180:ARG:NH1	2.46	0.49
2:F:352:ALA:HB3	2:F:353:PRO:HD3	1.95	0.49
6:K:32:ALA:HB1	6:L:34:ILE:HB	1.94	0.49
2:D:116:ILE:HG21	2:D:266:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:HG22	1:A:67:VAL:HG22	1.95	0.49
2:E:45:THR:HB	2:E:52:ASP:HB2	1.95	0.49
2:F:67:LEU:HB2	2:F:79:LEU:HB2	1.94	0.49
3:G:67:GLU:HB2	3:G:71:LYS:HB2	1.94	0.49
6:T:30:PHE:HA	6:T:33:LEU:HB3	1.94	0.49
1:A:438:ALA:HA	1:A:441:LYS:HE2	1.95	0.48
2:F:81:VAL:HA	2:F:92:THR:HG22	1.95	0.48
6:L:4:VAL:HG13	6:M:9:TYR:HE2	1.77	0.48
1:C:251:ALA:HA	1:C:254:TYR:CE2	2.48	0.48
6:S:5:LEU:HA	6:S:8:LYS:HD3	1.95	0.48
1:C:446:ARG:NH2	1:C:475:VAL:O	2.47	0.48
2:D:422:LEU:HD21	3:G:44:MET:HE1	1.95	0.48
6:R:3:LEU:HD21	6:S:3:LEU:HD13	1.96	0.48
1:A:423:TYR:HA	1:A:426:VAL:HG12	1.96	0.48
2:E:352:ALA:HB3	2:E:353:PRO:HD3	1.95	0.48
3:G:70:GLU:HA	3:G:73:PHE:HB3	1.95	0.48
6:K:26:ILE:HG23	6:K:55:PHE:HB2	1.96	0.48
6:L:68:ILE:HD11	6:M:66:LEU:HD12	1.96	0.48
1:A:462:MET:HB2	1:A:467:MET:HE3	1.95	0.48
2:E:68:THR:HB	2:E:76:LYS:HE2	1.96	0.48
2:F:419:ILE:HG23	2:F:424:MET:HG2	1.96	0.48
6:T:63:LEU:O	6:T:67:MET:N	2.47	0.48
2:E:436:GLU:O	2:E:440:LYS:HG2	2.14	0.47
1:B:52:ASN:HA	1:B:71:ASN:HB2	1.96	0.47
2:E:171:VAL:HG22	2:E:445:LEU:HD22	1.95	0.47
6:O:3:LEU:HD21	6:P:3:LEU:HD13	1.96	0.47
1:A:420:LEU:HA	1:A:423:TYR:HB3	1.96	0.47
1:B:423:TYR:CE1	1:B:424:ARG:HG3	2.49	0.47
1:B:379:GLU:HG3	1:B:381:GLU:H	1.79	0.47
2:D:268:LEU:HD21	2:D:326:ARG:HB2	1.97	0.47
6:Q:68:ILE:HD12	6:R:16:SER:HB3	1.97	0.47
1:A:190:ARG:O	1:A:373:ASP:N	2.46	0.47
1:A:353:ILE:HD11	1:A:368:VAL:HG21	1.97	0.47
2:E:173:ASP:HB3	2:E:465:LEU:HD13	1.96	0.47
6:K:28:ILE:HG22	6:L:31:ALA:HB2	1.96	0.47
6:L:4:VAL:HG23	6:M:2:GLN:HG3	1.97	0.47
6:O:68:ILE:HD11	6:P:66:LEU:HD12	1.97	0.47
1:A:165:ARG:NH2	1:A:333:GLU:O	2.47	0.47
2:D:191:GLY:HA2	9:D:600:ADP:H5'1	1.97	0.47
1:A:125:VAL:HG12	1:A:279:MET:HA	1.97	0.46
2:D:43:ILE:HD11	2:D:69:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:VAL:HG13	2:E:90:VAL:HG13	1.96	0.46
2:E:390:ASP:OD1	2:E:391:ILE:N	2.48	0.46
6:S:4:VAL:HG22	6:T:5:LEU:HB2	1.97	0.46
1:A:382:LEU:HB2	1:A:390:ALA:HB1	1.96	0.46
1:C:167:SER:OG	2:D:230:ARG:NE	2.48	0.46
2:D:116:ILE:HD11	2:D:269:THR:HB	1.97	0.46
2:F:286:VAL:HG11	2:F:289:ILE:HD13	1.96	0.46
2:F:441:ILE:HG23	2:F:472:PHE:HE2	1.79	0.46
2:D:433:LEU:HG	2:D:437:ARG:HE	1.81	0.46
2:F:63:ILE:HG22	2:F:64:LEU:HG	1.97	0.46
2:F:221:ARG:NH1	2:F:224:GLU:OE2	2.47	0.46
3:G:215:GLU:OE2	6:N:39:ARG:NH1	2.48	0.46
1:A:264:GLU:HB3	1:A:268:LEU:HD12	1.96	0.46
1:A:524:LYS:O	1:A:527:THR:OG1	2.33	0.46
2:E:183:LYS:HB3	2:E:360:LEU:HD23	1.97	0.46
6:K:9:TYR:HD2	6:T:8:LYS:HG2	1.79	0.46
3:G:61:THR:HG23	4:H:15:LEU:O	2.16	0.46
2:D:67:LEU:HD12	2:D:92:THR:HG21	1.98	0.46
6:M:63:LEU:O	6:M:67:MET:N	2.48	0.46
1:A:449:ARG:O	1:A:453:LEU:N	2.45	0.46
1:B:79:VAL:HG21	1:B:99:ILE:HD13	1.97	0.46
6:M:32:ALA:HA	6:M:35:ASN:HB3	1.98	0.46
2:E:318:THR:O	2:E:322:ALA:N	2.44	0.46
3:G:224:LEU:HA	4:H:73:PHE:HE2	1.81	0.46
6:S:28:ILE:HB	6:T:27:ALA:HB1	1.98	0.46
6:T:35:ASN:O	6:T:39:ARG:HG2	2.17	0.46
1:C:271:LEU:HG	1:C:275:THR:HG23	1.97	0.45
1:C:293:VAL:HG22	1:C:350:LEU:HB2	1.98	0.45
1:B:482:ILE:HD12	1:B:483:PRO:HD2	1.98	0.45
2:D:287:ASP:HA	2:D:288:ASN:HA	1.56	0.45
2:E:123:LEU:HD23	2:E:247:THR:HB	1.98	0.45
2:E:287:ASP:HA	2:E:288:ASN:HA	1.55	0.45
6:Q:3:LEU:HB3	6:R:2:GLN:HB3	1.97	0.45
1:A:162:ILE:O	2:E:226:ASN:ND2	2.49	0.45
6:K:34:ILE:HG21	6:T:33:LEU:HA	1.99	0.45
1:B:468:VAL:HG11	1:B:515:LEU:HD11	1.99	0.45
1:C:192:LEU:HA	1:C:351:PRO:HD2	1.99	0.45
2:D:183:LYS:NZ	2:D:324:GLN:HB3	2.30	0.45
1:A:170:GLU:HB2	1:A:187:ARG:HB2	1.97	0.45
1:A:216:ASN:HA	1:A:224:LYS:HD3	1.98	0.45
2:E:117:PRO:HA	2:E:144:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:ARG:NH1	2:D:77:LEU:HB2	2.31	0.45
2:D:185:GLY:HA2	2:D:339:GLN:O	2.16	0.45
1:B:116:ARG:HH21	1:B:118:GLY:HA2	1.81	0.45
1:C:356:GLN:HB3	2:F:349:THR:HG22	1.99	0.45
2:E:116:ILE:HD11	2:E:269:THR:HB	1.98	0.45
2:D:218:VAL:HG22	2:D:263:VAL:HG13	1.99	0.45
2:D:308:SER:OG	2:D:309:ALA:N	2.50	0.45
2:D:437:ARG:HH12	2:D:478:GLY:N	2.15	0.45
2:F:329:THR:HG23	2:F:334:SER:HA	1.99	0.45
6:K:57:LEU:HD13	6:L:55:PHE:CE1	2.52	0.45
6:S:10:ILE:HB	6:T:10:ILE:HG12	1.99	0.45
2:F:186:LEU:HB2	2:F:340:ALA:HA	1.99	0.44
4:H:36:GLU:N	6:Q:39:ARG:O	2.51	0.44
6:N:33:LEU:HA	6:O:34:ILE:HG21	1.99	0.44
1:A:70:LEU:HB3	1:A:73:ILE:HB	1.99	0.44
6:Q:7:GLY:HA2	6:R:10:ILE:HD11	1.98	0.44
1:A:399:ARG:NH1	2:E:190:ALA:HB3	2.32	0.44
1:B:173:GLN:O	1:B:211:ASN:ND2	2.50	0.44
1:B:465:GLU:HB3	1:B:506:LEU:HB3	2.00	0.44
2:E:181:GLY:HA3	2:E:329:THR:OG1	2.17	0.44
2:E:145:PHE:HD2	2:E:146:LEU:HG	1.82	0.44
6:M:5:LEU:HA	6:M:8:LYS:HD3	1.99	0.44
6:S:15:ALA:HB3	6:S:69:ALA:HB2	1.99	0.44
2:E:218:VAL:HG11	2:E:292:PHE:HB2	2.00	0.44
2:E:286:VAL:HG11	2:E:289:ILE:HD13	2.00	0.44
2:E:313:GLN:OE1	2:E:313:GLN:N	2.43	0.44
1:C:70:LEU:HD13	1:C:73:ILE:HD12	2.00	0.44
2:F:303:LEU:HD12	2:F:305:ARG:HH12	1.83	0.44
3:G:65:TYR:HD1	4:H:15:LEU:HD12	1.82	0.44
1:C:190:ARG:HH22	2:D:221:ARG:HB3	1.82	0.44
1:C:337:LYS:NZ	1:C:344:GLY:O	2.42	0.44
1:C:419:PHE:CE2	1:C:475:VAL:HG23	2.53	0.44
2:D:408:THR:HG22	2:D:438:ALA:HB2	2.00	0.44
6:R:27:ALA:O	6:R:31:ALA:N	2.46	0.44
2:F:218:VAL:HG22	2:F:263:VAL:HG13	1.98	0.44
1:A:72:ASN:O	1:A:116:ARG:NH1	2.50	0.43
1:B:125:VAL:HG21	1:B:153:ILE:HG13	1.98	0.43
2:D:275:ARG:NH1	2:D:276:ASP:OD1	2.51	0.43
2:E:310:VAL:H	3:G:279:THR:HG22	1.82	0.43
4:H:36:GLU:O	6:P:40:ASN:ND2	2.51	0.43
6:K:15:ALA:HB3	6:K:69:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ALA:HA	1:C:416:LEU:HB3	2.01	0.43
2:F:221:ARG:NH1	10:F:2003:HOH:O	2.50	0.43
3:G:183:TYR:HE1	3:G:197:LYS:HB2	1.83	0.43
1:A:51:LEU:O	1:A:71:ASN:ND2	2.48	0.43
2:D:69:ILE:HD12	2:D:77:LEU:HD23	2.01	0.43
2:E:382:LEU:HD21	2:E:409:LEU:HB2	2.00	0.43
3:G:67:GLU:HB2	3:G:71:LYS:HD3	2.00	0.43
6:K:24:ILE:O	6:K:28:ILE:HG13	2.19	0.43
6:M:24:ILE:O	6:M:28:ILE:HG13	2.18	0.43
1:A:205:ALA:HB1	1:A:293:VAL:HG11	1.99	0.43
1:B:232:VAL:HG11	1:B:300:GLN:HB2	1.99	0.43
1:C:170:GLU:OE2	1:C:337:LYS:NZ	2.44	0.43
1:C:431:GLN:OE1	1:C:431:GLN:N	2.52	0.43
6:K:4:VAL:HG13	6:L:9:TYR:HE2	1.84	0.43
6:P:43:LEU:HD12	6:Q:38:SER:HA	1.99	0.43
1:A:267:PRO:HA	1:A:307:MET:HE1	2.01	0.42
1:C:399:ARG:HE	9:D:600:ADP:H5'2	1.84	0.42
2:E:126:ILE:HG23	2:E:250:PHE:HD2	1.83	0.42
2:F:167:THR:HA	2:F:205:ILE:HD11	2.00	0.42
4:H:15:LEU:HD22	4:H:89:ALA:HB2	2.01	0.42
6:R:33:LEU:HD21	6:R:48:PHE:HE1	1.83	0.42
1:C:367:ASN:O	1:C:371:ILE:HG13	2.19	0.42
2:F:275:ARG:HD3	2:F:335:VAL:HG23	2.00	0.42
6:L:57:LEU:HD13	6:M:55:PHE:CZ	2.54	0.42
1:B:279:MET:HE2	1:B:279:MET:HB3	1.82	0.42
1:B:281:GLU:HG3	1:B:284:ARG:HE	1.85	0.42
2:D:202:ILE:HG21	2:D:232:MET:HE1	2.01	0.42
1:A:102:PHE:CE2	1:A:137:LEU:HD21	2.53	0.42
1:B:155:ALA:O	1:B:334:ARG:NH1	2.52	0.42
2:D:71:ARG:HH12	2:D:77:LEU:HB2	1.84	0.42
1:A:177:LYS:HE2	1:A:177:LYS:HB3	1.84	0.42
1:B:497:TYR:HE2	1:B:526:ILE:HD11	1.84	0.42
3:G:94:SER:HB2	3:G:153:GLY:HA3	2.02	0.42
6:T:24:ILE:O	6:T:28:ILE:HG13	2.20	0.42
1:C:409:MET:O	1:C:413:ALA:N	2.46	0.42
6:P:8:LYS:HB3	6:P:72:LEU:O	2.20	0.42
1:B:91:ASN:HB3	2:F:47:ILE:HG23	2.01	0.42
1:B:295:ASP:HA	1:B:296:ASP:HA	1.79	0.42
6:N:68:ILE:HD11	6:O:66:LEU:HD12	2.01	0.42
1:C:91:ASN:HB2	2:D:47:ILE:HG12	2.01	0.42
2:D:265:LEU:HD23	2:D:323:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:ILE:HB	2:F:77:LEU:HB3	2.01	0.42
6:S:58:SER:O	6:S:61:THR:OG1	2.36	0.42
6:K:27:ALA:HA	6:K:30:PHE:CE2	2.54	0.42
6:Q:11:GLY:HA2	6:Q:14:LEU:HD12	2.02	0.42
1:A:163:LEU:C	1:A:165:ARG:H	2.28	0.41
1:B:232:VAL:HG21	1:B:273:PRO:HG3	2.01	0.41
1:B:306:GLN:NE2	2:E:315:THR:HG22	2.34	0.41
2:E:174:LEU:HA	2:E:398:HIS:CE1	2.54	0.41
2:E:183:LYS:HB2	2:E:360:LEU:HA	2.00	0.41
2:E:327:ILE:HG21	2:E:337:SER:HB2	2.02	0.41
2:E:473:LYS:HE2	2:E:473:LYS:HB3	1.87	0.41
6:M:32:ALA:HB1	6:N:34:ILE:HB	2.02	0.41
1:C:525:SER:O	1:C:529:ASN:ND2	2.54	0.41
2:E:183:LYS:HE2	2:E:324:GLN:HB3	2.02	0.41
3:G:73:PHE:HZ	3:G:205:ILE:HG12	1.85	0.41
2:D:81:VAL:HA	2:D:92:THR:HG22	2.02	0.41
6:O:8:LYS:HE2	6:O:73:LEU:HA	2.02	0.41
1:B:209:ILE:O	1:B:254:TYR:OH	2.33	0.41
2:F:237:VAL:HG13	2:F:245:LYS:HB3	2.02	0.41
6:P:26:ILE:HG23	6:P:55:PHE:HB2	2.02	0.41
6:P:68:ILE:HD12	6:Q:16:SER:HB3	2.02	0.41
2:E:427:LEU:HD22	2:E:431:ASP:HB3	2.02	0.41
2:F:185:GLY:HA3	2:F:360:LEU:HD13	2.02	0.41
2:D:478:GLY:HA2	2:D:481:ASP:HB2	2.01	0.41
2:F:69:ILE:HD11	2:F:79:LEU:HD11	2.01	0.41
2:F:498:VAL:HA	2:F:501:ALA:HB3	2.01	0.41
1:C:229:TYR:OH	1:C:295:ASP:OD2	2.26	0.41
2:D:412:TYR:CE1	2:D:435:VAL:HG13	2.56	0.41
6:P:28:ILE:HG22	6:Q:31:ALA:HB2	2.01	0.41
1:B:193:ILE:HB	1:B:352:ILE:HG12	2.03	0.41
1:C:91:ASN:HD21	1:C:311:LEU:HB3	1.85	0.41
1:A:313:ARG:HA	1:A:314:PRO:HD3	1.98	0.41
1:B:70:LEU:HD22	1:B:116:ARG:HG3	2.03	0.41
1:B:168:VAL:HG12	1:B:337:LYS:HB3	2.02	0.41
1:B:213:LYS:NZ	1:B:249:HIS:HB3	2.36	0.41
1:B:295:ASP:HB2	1:B:352:ILE:HD12	2.03	0.41
1:C:373:ASP:CG	2:D:223:ARG:HE	2.28	0.41
2:D:209:HIS:NE2	2:D:281:ASP:O	2.40	0.41
2:D:377:PRO:HB2	2:D:379:VAL:HG23	2.03	0.41
2:E:268:LEU:HD13	2:E:284:LEU:HD22	2.02	0.41
2:E:488:PHE:HE1	2:E:497:VAL:HG11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:32:SER:HA	4:H:50:LEU:HA	2.02	0.41
4:H:45:PRO:HG3	4:H:78:PRO:HD3	2.02	0.41
6:O:57:LEU:HD13	6:P:55:PHE:CE2	2.55	0.41
6:S:32:ALA:O	6:S:36:GLY:N	2.54	0.41
1:A:91:ASN:HD21	1:A:311:LEU:HD22	1.86	0.41
1:B:182:LEU:HD22	1:B:417:LYS:HB2	2.03	0.41
1:C:187:ARG:NH2	1:C:225:LEU:HB2	2.36	0.41
2:E:119:GLY:HA2	2:E:273:TYR:CE2	2.56	0.41
2:E:165:LEU:HB2	2:E:180:ARG:HB2	2.03	0.41
2:F:194:LYS:HE3	2:F:342:TYR:HA	2.03	0.41
2:F:228:LEU:O	2:F:232:MET:HG2	2.21	0.41
3:G:78:THR:HB	3:G:204:ALA:O	2.21	0.41
6:M:57:LEU:HD13	6:N:55:PHE:CE2	2.56	0.41
6:S:54:GLY:HA2	6:T:30:PHE:CD1	2.56	0.41
1:B:133:VAL:HB	1:B:142:ASP:HB3	2.03	0.40
2:F:245:LYS:HE2	2:F:245:LYS:HB2	1.93	0.40
3:G:51:LYS:O	3:G:55:ALA:N	2.53	0.40
6:P:28:ILE:HB	6:Q:27:ALA:HB1	2.02	0.40
6:Q:24:ILE:O	6:Q:28:ILE:HG13	2.21	0.40
6:R:33:LEU:HD21	6:R:48:PHE:CE1	2.56	0.40
2:D:146:LEU:HA	2:D:147:PRO:HD3	1.96	0.40
2:F:46:VAL:HG22	2:F:51:VAL:HG13	2.03	0.40
3:G:248:ARG:O	3:G:252:MET:HG2	2.21	0.40
4:H:32:SER:HA	4:H:50:LEU:HD23	2.02	0.40
6:R:57:LEU:HB2	6:S:26:ILE:HG21	2.02	0.40
1:C:386:GLY:O	1:C:455:LYS:HE2	2.20	0.40
2:E:474:GLU:O	2:E:479:LYS:HB2	2.21	0.40
2:F:196:VAL:HG23	9:F:600:ADP:O1A	2.22	0.40
1:B:264:GLU:HB3	1:B:268:LEU:HD12	2.03	0.40
2:D:213:SER:HB2	2:D:246:VAL:HG23	2.03	0.40
2:E:145:PHE:CD2	2:E:146:LEU:HG	2.57	0.40
2:F:287:ASP:HA	2:F:288:ASN:HA	1.56	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	483/536 (90%)	456 (94%)	26 (5%)	1 (0%)	43	74
1	B	475/536 (89%)	454 (96%)	21 (4%)	0	100	100
1	C	483/536 (90%)	456 (94%)	27 (6%)	0	100	100
2	D	468/509 (92%)	448 (96%)	20 (4%)	0	100	100
2	E	466/509 (92%)	443 (95%)	23 (5%)	0	100	100
2	F	468/509 (92%)	439 (94%)	28 (6%)	1 (0%)	43	74
3	G	263/293 (90%)	242 (92%)	21 (8%)	0	100	100
4	H	109/137 (80%)	92 (84%)	13 (12%)	4 (4%)	2	21
6	K	71/76 (93%)	71 (100%)	0	0	100	100
6	L	70/76 (92%)	67 (96%)	3 (4%)	0	100	100
6	M	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
6	N	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
6	O	73/76 (96%)	73 (100%)	0	0	100	100
6	P	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
6	Q	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	R	72/76 (95%)	72 (100%)	0	0	100	100
6	S	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
6	T	72/76 (95%)	71 (99%)	1 (1%)	0	100	100
All	All	3938/4325 (91%)	3739 (95%)	193 (5%)	6 (0%)	43	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	75	ASN
4	H	120	ALA
4	H	45	PRO
1	A	400	VAL
4	H	78	PRO
4	H	118	VAL

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	391/429 (91%)	388 (99%)	3 (1%)	73	77
1	B	387/429 (90%)	380 (98%)	7 (2%)	51	69
1	C	391/429 (91%)	391 (100%)	0	100	100
2	D	377/409 (92%)	377 (100%)	0	100	100
2	E	376/409 (92%)	376 (100%)	0	100	100
2	F	377/409 (92%)	375 (100%)	2 (0%)	81	80
3	G	224/242 (93%)	222 (99%)	2 (1%)	70	76
4	H	92/114 (81%)	92 (100%)	0	100	100
6	K	50/52 (96%)	50 (100%)	0	100	100
6	L	49/52 (94%)	49 (100%)	0	100	100
6	M	51/52 (98%)	51 (100%)	0	100	100
6	N	51/52 (98%)	50 (98%)	1 (2%)	48	67
6	O	51/52 (98%)	48 (94%)	3 (6%)	18	44
6	P	51/52 (98%)	50 (98%)	1 (2%)	48	67
6	Q	52/52 (100%)	52 (100%)	0	100	100
6	R	50/52 (96%)	49 (98%)	1 (2%)	48	67
6	S	50/52 (96%)	49 (98%)	1 (2%)	48	67
6	T	50/52 (96%)	48 (96%)	2 (4%)	28	54
All	All	3120/3390 (92%)	3097 (99%)	23 (1%)	76	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	270	TYR
1	A	480	ASP
1	B	60	VAL
1	B	100	VAL
1	B	234	GLN

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Mol	Chain	Res	Type
1	B	270	TYR
1	B	423	TYR
1	B	445	THR
1	B	465	GLU
2	F	293	THR
2	F	451	VAL
3	G	78	THR
3	G	176	TYR
6	N	55	PHE
6	O	55	PHE
6	O	71	LEU
6	O	73	LEU
6	P	1	MET
6	R	55	PHE
6	S	55	PHE
6	T	34	ILE
6	T	55	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	501	ASN
1	B	72	ASN
1	B	442	GLN
1	C	203	GLN
1	C	286	ASN
1	C	529	ASN
2	D	324	GLN
2	D	416	GLN
2	E	480	HIS
2	F	88	ASN
2	F	359	HIS
6	R	35	ASN
6	S	2	GLN
6	S	46	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
7	ATP	A	600	8	32,33,33	1.40	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	C	600	8	32,33,33	1.91	5 (15%)	48,52,52	1.75	9 (18%)
9	ADP	F	600	8	28,29,29	1.41	4 (14%)	43,45,45	1.84	8 (18%)
7	ATP	B	600	8	32,33,33	1.42	4 (12%)	48,52,52	1.76	9 (18%)
9	ADP	D	600	8	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	A	600	8	-	0/22/38/38	0/3/3/3
7	ATP	C	600	8	-	1/22/38/38	0/3/3/3
9	ADP	F	600	8	-	3/16/32/32	0/3/3/3
7	ATP	B	600	8	-	0/22/38/38	0/3/3/3
9	ADP	D	600	8	-	2/16/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	600	ATP	PB-O3A	-7.48	1.51	1.59
7	A	600	ATP	C5-C4	4.79	1.47	1.39
7	B	600	ATP	C5-C4	4.77	1.47	1.39
9	F	600	ADP	C5-C4	4.73	1.47	1.39
7	C	600	ATP	C5-C4	4.73	1.47	1.39
9	D	600	ADP	C5-C4	4.73	1.47	1.39
9	D	600	ADP	C5-C6	2.76	1.48	1.41
7	A	600	ATP	C5-C6	2.75	1.48	1.41
7	C	600	ATP	C5-C6	2.75	1.48	1.41
7	B	600	ATP	C5-C6	2.75	1.48	1.41
9	F	600	ADP	C5-C6	2.70	1.48	1.41
7	C	600	ATP	C8-N7	2.35	1.36	1.31
9	D	600	ADP	C8-N7	2.34	1.36	1.31
7	B	600	ATP	C8-N7	2.33	1.36	1.31
7	A	600	ATP	C8-N7	2.33	1.36	1.31
9	F	600	ADP	C8-N7	2.31	1.36	1.31
9	D	600	ADP	C5-N7	-2.31	1.34	1.39
9	F	600	ADP	C5-N7	-2.31	1.34	1.39
7	B	600	ATP	C5-N7	-2.28	1.34	1.39
7	C	600	ATP	C5-N7	-2.27	1.34	1.39
7	A	600	ATP	C5-N7	-2.25	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	600	ADP	C5-C4-N3	-5.89	118.61	126.72
7	B	600	ATP	C5-C4-N3	-5.87	118.64	126.72
7	A	600	ATP	C5-C4-N3	-5.83	118.69	126.72
7	C	600	ATP	C5-C4-N3	-5.80	118.74	126.72
9	D	600	ADP	C5-C4-N3	-5.76	118.78	126.72
9	F	600	ADP	N3-C4-N9	4.75	135.24	127.17
7	A	600	ATP	N3-C4-N9	4.68	135.12	127.17
7	B	600	ATP	N3-C4-N9	4.65	135.07	127.17
9	D	600	ADP	N3-C4-N9	4.61	135.00	127.17
7	C	600	ATP	N3-C4-N9	4.59	134.98	127.17
9	F	600	ADP	C2-N3-C4	3.70	120.86	111.83
7	A	600	ATP	C2-N3-C4	3.69	120.85	111.83
7	B	600	ATP	C2-N3-C4	3.69	120.85	111.83
7	C	600	ATP	C2-N3-C4	3.68	120.81	111.83
9	D	600	ADP	C2-N3-C4	3.68	120.81	111.83
7	C	600	ATP	C4-C5-N7	-3.45	106.64	110.58
7	B	600	ATP	C4-C5-N7	-3.44	106.64	110.58
7	A	600	ATP	C4-C5-N7	-3.42	106.67	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	600	ADP	C4-C5-N7	-3.41	106.68	110.58
9	F	600	ADP	C4-C5-N7	-3.31	106.80	110.58
9	D	600	ADP	N3-C2-N1	-3.25	123.66	128.58
7	A	600	ATP	N3-C2-N1	-3.23	123.70	128.58
7	B	600	ATP	N3-C2-N1	-3.21	123.72	128.58
7	C	600	ATP	N3-C2-N1	-3.21	123.73	128.58
9	F	600	ADP	N3-C2-N1	-3.19	123.76	128.58
7	A	600	ATP	C4-N9-C8	2.66	108.53	105.74
7	C	600	ATP	C4-N9-C8	2.65	108.52	105.74
9	D	600	ADP	C4-N9-C8	2.64	108.51	105.74
7	B	600	ATP	C4-N9-C8	2.56	108.43	105.74
9	F	600	ADP	C4-N9-C8	2.55	108.42	105.74
7	A	600	ATP	C5-N7-C8	2.54	107.44	103.45
7	C	600	ATP	C5-N7-C8	2.52	107.42	103.45
9	D	600	ADP	C5-N7-C8	2.52	107.41	103.45
7	B	600	ATP	C5-N7-C8	2.51	107.40	103.45
9	F	600	ADP	C3'-C2'-C1'	2.47	106.14	101.46
9	D	600	ADP	C3'-C2'-C1'	2.46	106.11	101.46
7	B	600	ATP	C3'-C2'-C1'	2.43	106.07	101.46
9	F	600	ADP	C5-N7-C8	2.42	107.25	103.45
7	C	600	ATP	C3'-C2'-C1'	2.25	105.73	101.46
7	A	600	ATP	C3'-C2'-C1'	2.20	105.62	101.46
7	C	600	ATP	C6-C5-N7	2.09	136.12	132.09
9	D	600	ADP	C6-C5-N7	2.08	136.10	132.09
7	A	600	ATP	C6-C5-N7	2.06	136.06	132.09
7	B	600	ATP	C6-C5-N7	2.04	136.03	132.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

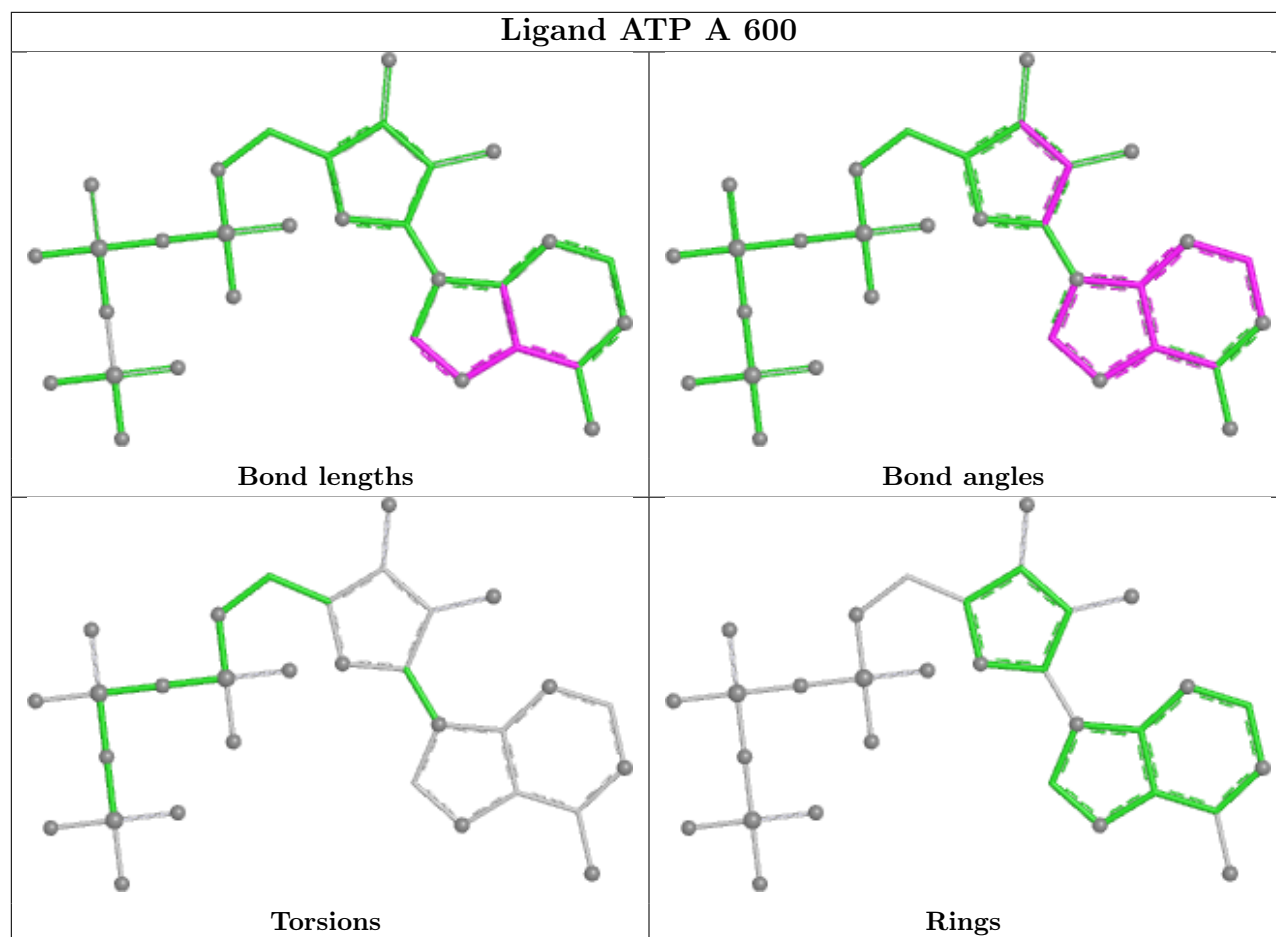
Mol	Chain	Res	Type	Atoms
9	F	600	ADP	C5'-O5'-PA-O2A
9	F	600	ADP	O4'-C4'-C5'-O5'
9	D	600	ADP	O4'-C4'-C5'-O5'
9	F	600	ADP	C3'-C4'-C5'-O5'
9	D	600	ADP	C3'-C4'-C5'-O5'
7	C	600	ATP	PG-O3B-PB-O2B

There are no ring outliers.

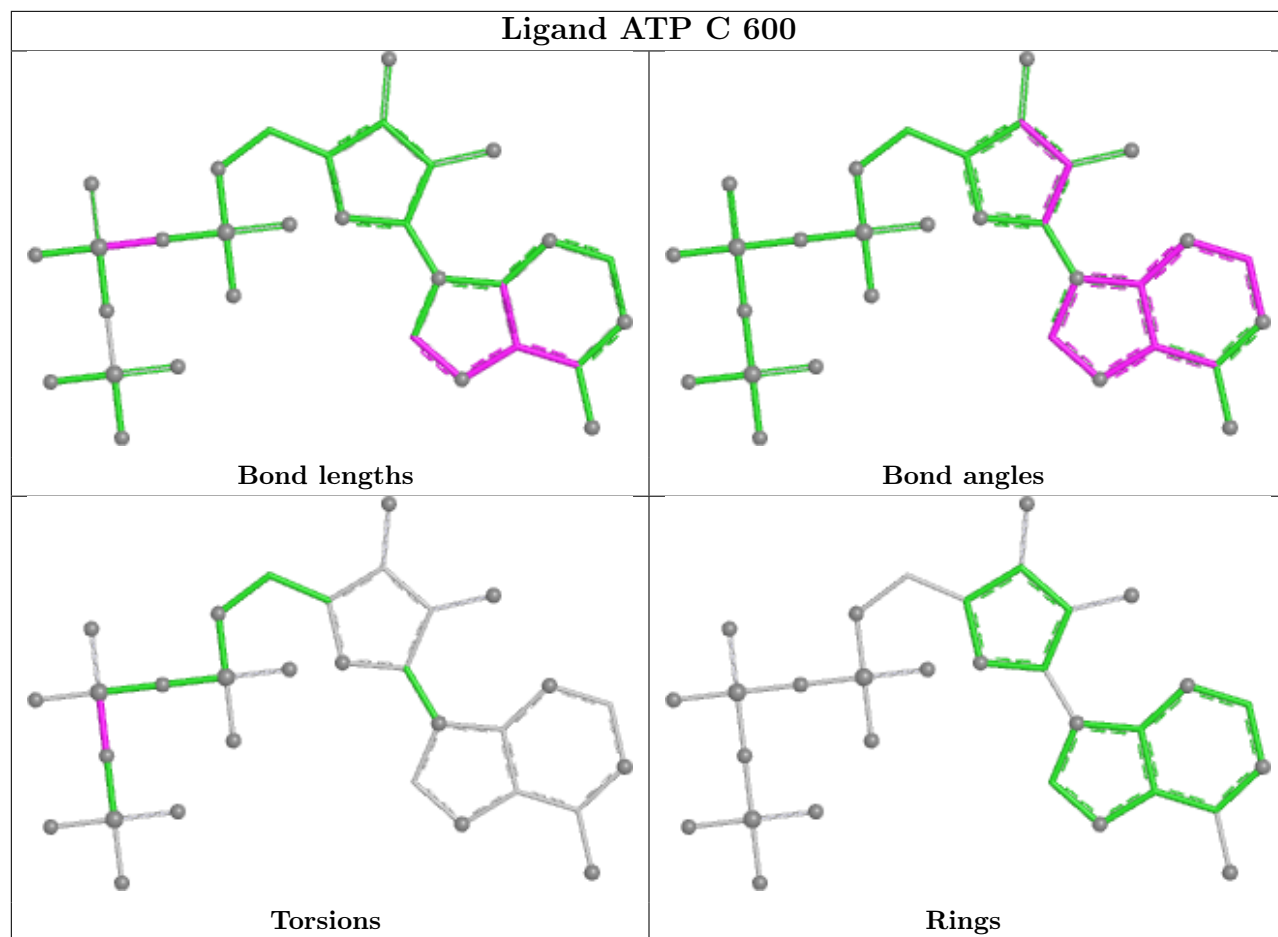
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	600	ATP	2	0
9	F	600	ADP	3	0
9	D	600	ADP	3	0

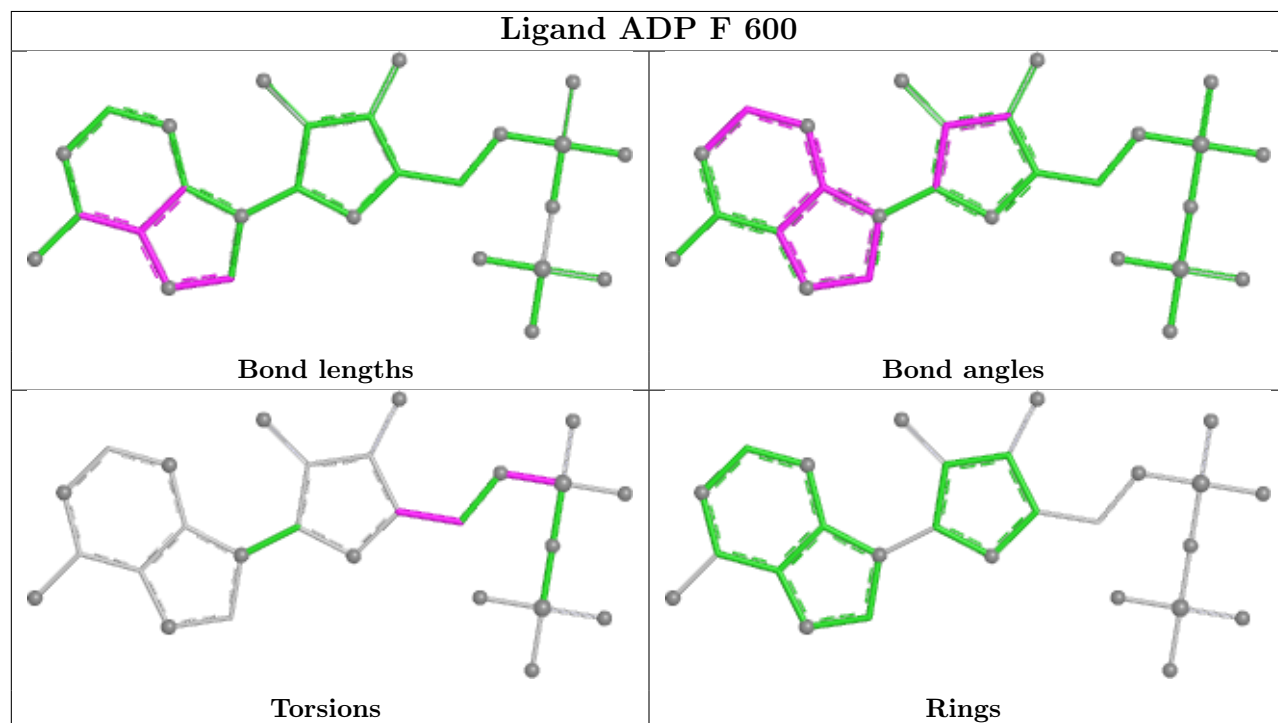
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



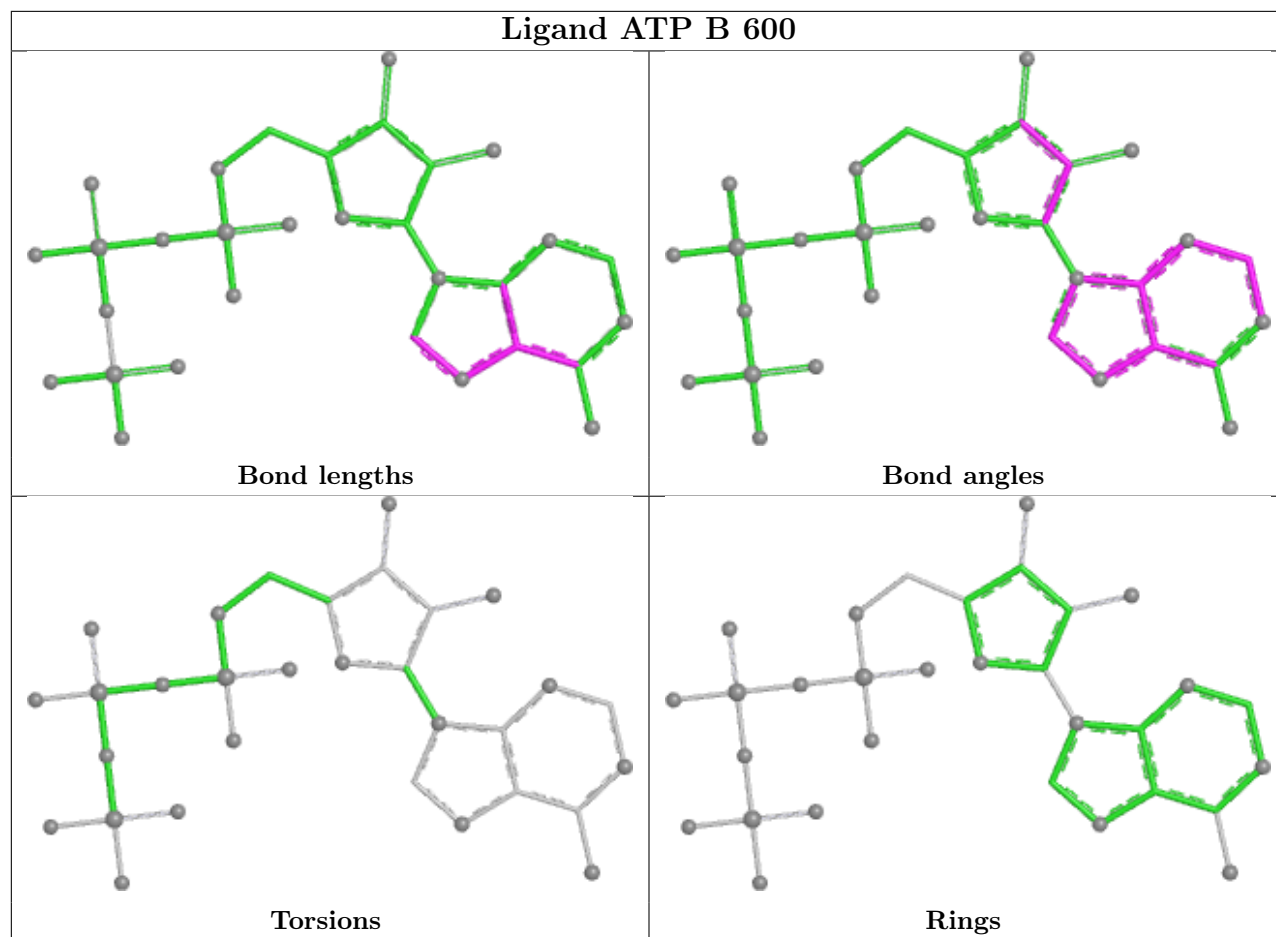
Ligand ATP C 600



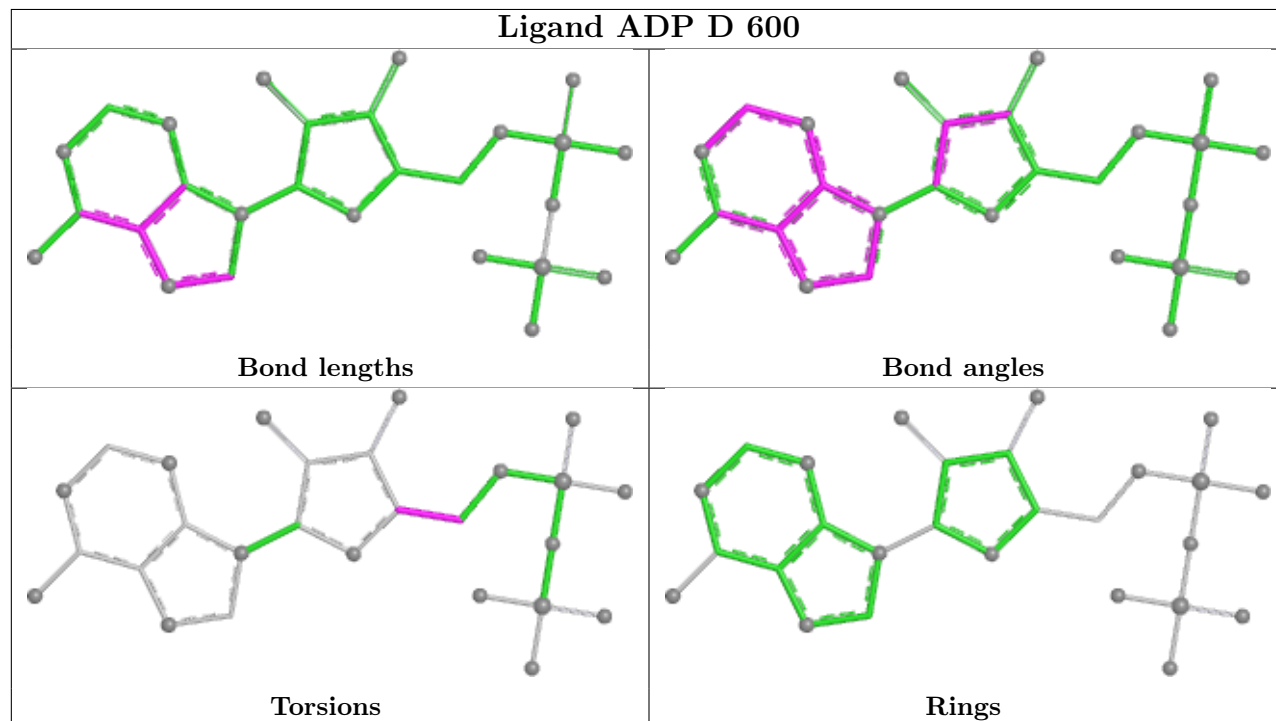
Ligand ADP F 600



Ligand ATP B 600



Ligand ADP D 600



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	485/536 (90%)	0.01	14 (2%)	53	31	116, 153, 209, 224	0
1	B	479/536 (89%)	0.07	16 (3%)	49	28	104, 156, 234, 261	0
1	C	485/536 (90%)	0.13	25 (5%)	33	19	108, 150, 222, 280	0
2	D	470/509 (92%)	0.19	21 (4%)	38	20	108, 158, 195, 215	0
2	E	468/509 (91%)	0.03	21 (4%)	38	20	117, 160, 210, 248	0
2	F	470/509 (92%)	0.07	18 (3%)	44	24	113, 152, 192, 213	0
3	G	267/293 (91%)	-0.04	8 (2%)	52	30	109, 185, 224, 241	0
4	H	113/137 (82%)	0.09	5 (4%)	39	21	161, 207, 255, 277	0
5	I	0/16	-	-	-	-	-	-
6	K	73/76 (96%)	0.73	8 (10%)	10	7	148, 184, 206, 218	0
6	L	72/76 (94%)	0.67	7 (9%)	13	9	154, 180, 213, 224	0
6	M	75/76 (98%)	0.54	6 (8%)	18	12	152, 179, 200, 213	0
6	N	75/76 (98%)	0.49	7 (9%)	14	9	140, 157, 188, 194	0
6	O	75/76 (98%)	0.33	3 (4%)	42	23	132, 158, 186, 192	0
6	P	75/76 (98%)	0.24	4 (5%)	32	18	132, 160, 200, 205	0
6	Q	76/76 (100%)	0.25	5 (6%)	24	15	150, 177, 198, 204	0
6	R	74/76 (97%)	0.13	6 (8%)	18	12	162, 182, 197, 213	0
6	S	74/76 (97%)	0.76	10 (13%)	7	5	164, 179, 203, 217	0
6	T	74/76 (97%)	0.59	6 (8%)	18	12	163, 182, 205, 210	0
All	All	3980/4341 (91%)	0.15	190 (4%)	35	19	104, 163, 216, 280	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	396	GLN	8.0
6	S	4	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
2	E	400	ASP	7.2
2	F	451	VAL	7.0
6	P	52	ILE	6.9
6	K	52	ILE	6.6
6	K	56	ALA	6.3
2	F	450	THR	6.1
2	D	178	TYR	6.1
6	L	24	ILE	5.9
1	B	402	SER	5.9
6	L	20	VAL	5.8
2	F	453	GLU	5.7
2	D	94	ALA	5.3
6	Q	63	LEU	5.2
6	T	63	LEU	5.1
1	C	62	ASP	5.0
2	E	173	ASP	4.9
6	M	17	ILE	4.9
2	E	391	ILE	4.8
2	E	393	VAL	4.8
1	A	219	GLN	4.7
6	K	17	ILE	4.7
4	H	39	ILE	4.6
2	E	174	LEU	4.5
6	M	20	VAL	4.4
6	N	17	ILE	4.4
6	S	3	LEU	4.3
2	E	399	TYR	4.3
6	N	3	LEU	4.2
1	C	413	ALA	4.2
2	E	390	ASP	4.1
2	F	454	VAL	4.1
6	L	52	ILE	4.1
6	P	49	THR	4.0
2	D	453	GLU	3.9
2	F	231	GLU	3.9
3	G	26	GLU	3.9
2	E	455	PHE	3.8
2	D	51	VAL	3.8
2	F	199	GLN	3.8
2	F	149	HIS	3.8
1	B	460	SER	3.7
2	D	339	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	108	VAL	3.7
1	C	403	ALA	3.7
1	B	459	ALA	3.6
6	P	53	LEU	3.5
6	T	60	ALA	3.5
1	A	156	GLN	3.4
2	F	372	GLU	3.4
6	K	20	VAL	3.4
2	D	96	ASP	3.4
6	T	52	ILE	3.3
1	B	360	VAL	3.3
6	L	17	ILE	3.3
4	H	27	GLN	3.3
1	C	402	SER	3.3
1	C	459	ALA	3.3
3	G	25	ARG	3.3
6	P	42	ALA	3.3
2	E	392	ASP	3.2
6	S	2	GLN	3.2
1	C	60	VAL	3.2
1	B	457	LYS	3.2
6	M	24	ILE	3.1
2	D	167	THR	3.1
6	K	53	LEU	3.1
2	D	450	THR	3.1
1	C	310	LEU	3.1
2	E	401	VAL	3.1
2	E	164	VAL	3.0
6	Q	70	PHE	3.0
2	F	64	LEU	3.0
6	Q	67	MET	3.0
6	N	24	ILE	3.0
6	M	52	ILE	3.0
2	D	95	MET	3.0
6	O	56	ALA	2.9
2	F	83	GLN	2.9
6	O	42	ALA	2.9
1	A	380	ALA	2.8
1	C	65	ALA	2.8
6	N	20	VAL	2.8
1	C	319	ALA	2.8
1	B	101	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	491	GLU	2.8
2	F	392	ASP	2.7
6	N	1	MET	2.7
2	D	176	ALA	2.7
4	H	46	THR	2.7
1	B	61	GLY	2.7
2	E	394	VAL	2.7
6	S	70	PHE	2.6
1	C	401	GLY	2.6
2	D	338	VAL	2.6
1	C	61	GLY	2.6
2	F	455	PHE	2.6
1	C	405	GLN	2.6
3	G	259	ALA	2.6
1	C	191	GLU	2.6
2	D	69	ILE	2.6
1	B	394	GLY	2.6
1	A	101	LEU	2.6
3	G	29	MET	2.6
6	T	56	ALA	2.6
1	A	391	ILE	2.5
1	C	90	LEU	2.5
6	Q	71	LEU	2.5
1	C	510	ALA	2.5
6	L	18	GLY	2.5
6	S	68	ILE	2.5
6	T	59	GLU	2.5
6	N	52	ILE	2.5
6	Q	17	ILE	2.5
6	O	63	LEU	2.5
6	K	55	PHE	2.4
2	F	225	GLY	2.4
2	E	398	HIS	2.4
2	D	204	ASN	2.4
1	B	58	LEU	2.4
6	R	3	LEU	2.4
6	S	5	LEU	2.4
1	A	275	THR	2.4
6	N	49	THR	2.4
2	E	348	LEU	2.4
1	C	178	ALA	2.4
6	L	22	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	395	GLY	2.4
1	A	459	ALA	2.3
2	E	402	ALA	2.3
2	E	177	PRO	2.3
2	E	251	GLY	2.3
6	R	20	VAL	2.3
2	D	184	ILE	2.3
3	G	283	VAL	2.3
2	D	85	LEU	2.3
1	C	221	GLU	2.3
2	D	203	ASN	2.3
1	C	105	ASP	2.3
1	C	315	PRO	2.3
2	D	451	VAL	2.3
1	B	462	MET	2.3
2	F	203	ASN	2.3
2	D	50	VAL	2.3
1	C	515	LEU	2.2
4	H	41	ALA	2.2
1	A	376	ILE	2.2
1	B	206	ILE	2.2
6	S	74	TYR	2.2
1	A	378	LEU	2.2
4	H	56	GLU	2.2
6	R	52	ILE	2.2
6	M	63	LEU	2.2
6	R	63	LEU	2.2
1	C	406	VAL	2.2
1	B	479	ILE	2.2
1	C	220	ASP	2.2
2	F	156	ALA	2.2
6	S	22	ALA	2.2
1	B	458	GLN	2.2
2	F	249	VAL	2.2
6	M	22	ALA	2.1
3	G	290	SER	2.1
6	K	18	GLY	2.1
6	K	21	GLY	2.1
6	R	53	LEU	2.1
2	D	420	ALA	2.1
1	B	212	GLN	2.1
3	G	286	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
6	S	52	ILE	2.1
1	A	381	GLU	2.1
2	F	452	ALA	2.1
1	A	155	ALA	2.1
3	G	281	GLU	2.1
6	T	17	ILE	2.1
6	L	46	GLN	2.1
1	C	176	LEU	2.1
2	E	85	LEU	2.1
6	R	50	TYR	2.1
1	A	220	ASP	2.1
1	A	473	ALA	2.1
2	E	490	MET	2.1
1	C	422	GLN	2.0
2	D	216	CYS	2.0
1	A	218	GLY	2.0
2	F	265	LEU	2.0
6	S	71	LEU	2.0
2	D	197	PHE	2.0
1	C	421	ALA	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 oligosaccharides 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
7	ATP	B	600	31/31	0.92	0.09	149,182,193,201	0
9	ADP	F	600	27/27	0.92	0.09	159,176,182,186	0
7	ATP	C	600	31/31	0.93	0.08	149,159,174,183	0

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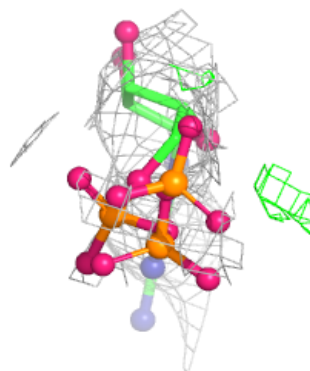
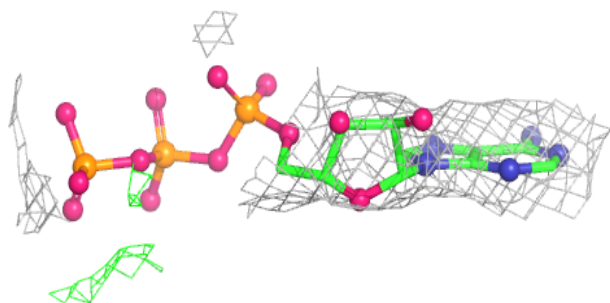
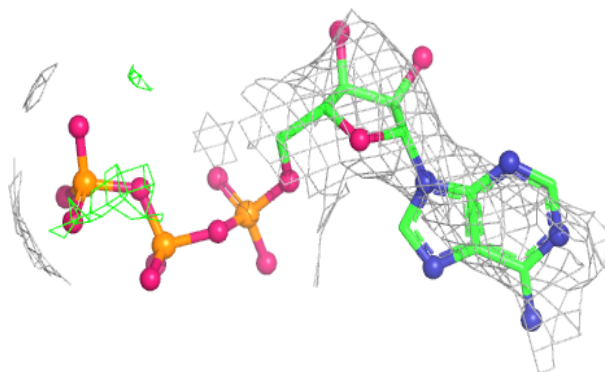
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	F	601	1/1	0.94	0.05	189,189,189,189	0
8	MG	C	601	1/1	0.94	0.08	171,171,171,171	0
8	MG	D	601	1/1	0.95	0.06	183,183,183,183	0
8	MG	A	601	1/1	0.95	0.05	173,173,173,173	0
9	ADP	D	600	27/27	0.95	0.07	159,164,170,173	0
7	ATP	A	600	31/31	0.95	0.06	146,160,172,197	0
8	MG	B	601	1/1	0.98	0.04	154,154,154,154	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.

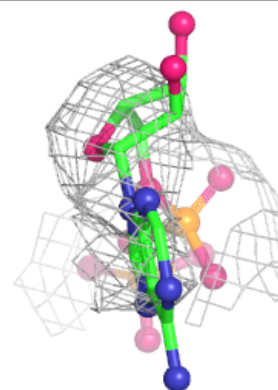
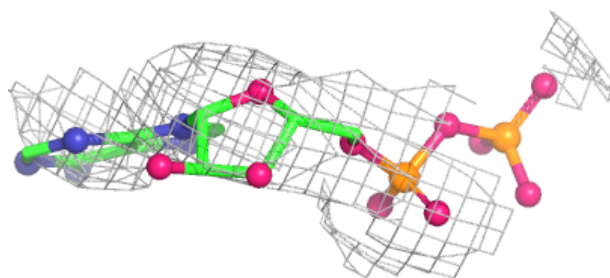
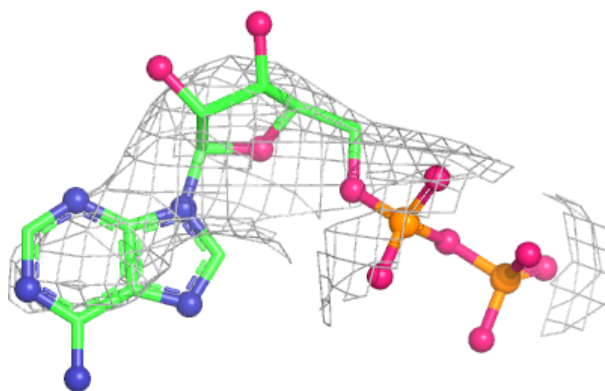
Electron density around ATP B 600:

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

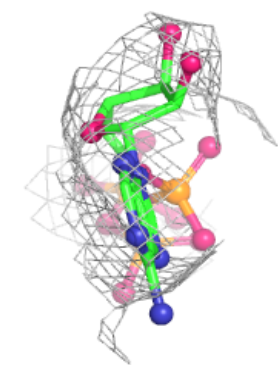
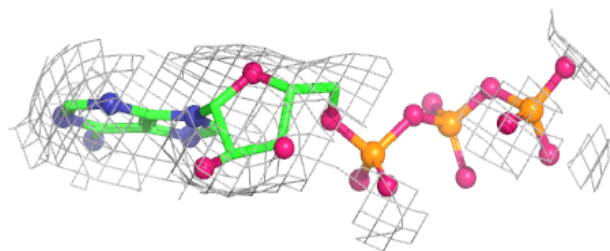
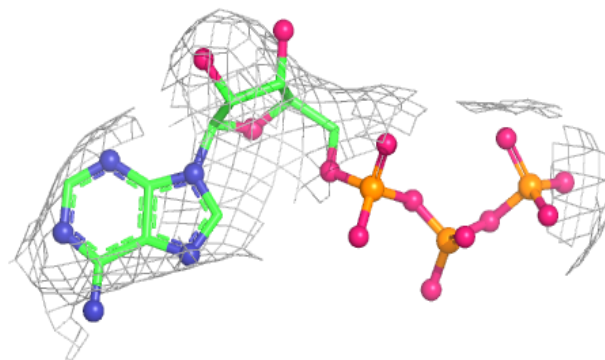


Electron density around ADP F 600:

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

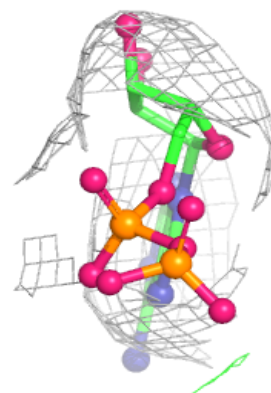
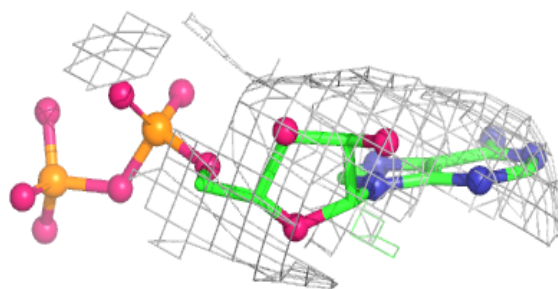
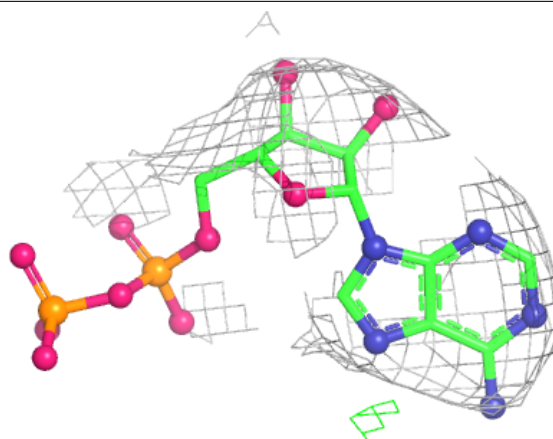
**Electron density around ATP C 600:**

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

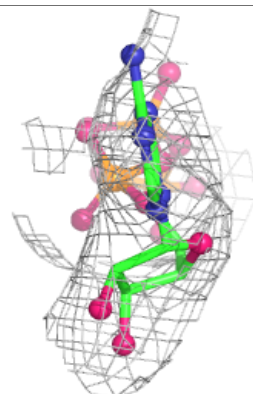
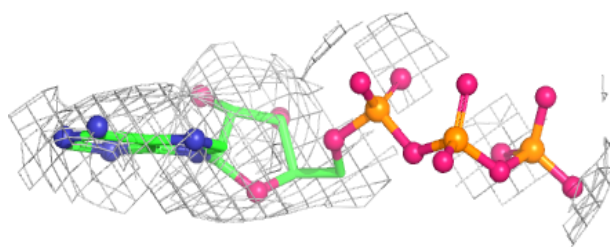
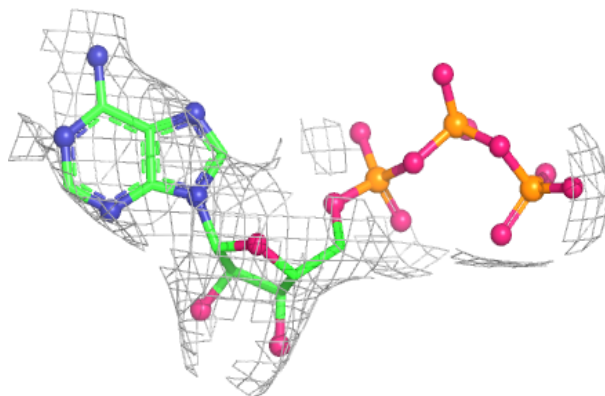


Electron density around ADP D 600:

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

**Electron density around ATP A 600:**

$2mF_o-DF_c$ (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.