



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 5JJK / pdb_00005jjk
Title : Rho transcription termination factor bound to rA7 and 6 ADP-BeF3 molecules
Authors : Thomsen, N.D.; Lawson, M.R.; Witkowsky, L.B.; Qu, S.; Berger, J.M.
Deposited on : 2016-04-24
Resolution : 3.15 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

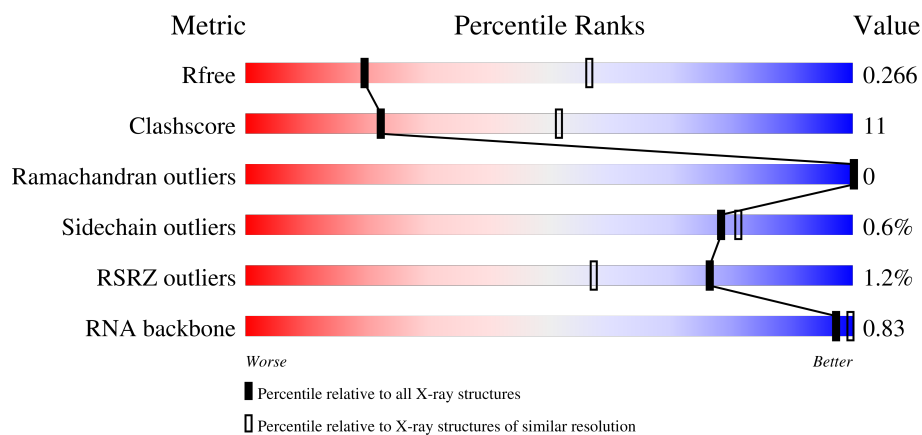
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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 $\leq 5\%$. 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	420	
1	B	420	
1	C	420	
1	D	420	

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Mol	Chain	Length	Quality of chain
1	E	420	3% 60% 25% 15%
1	F	420	% 64% 29% 7%
2	G	12	33% 25% 42%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19062 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	Se	0	0	0
			3181	2006	560	599	1	15			
1	B	409	Total	C	N	O	S	Se	0	0	0
			3219	2028	569	606	1	15			
1	C	411	Total	C	N	O	S	Se	0	0	0
			3231	2035	571	608	1	16			
1	D	405	Total	C	N	O	S	Se	0	0	0
			3181	2005	560	600	1	15			
1	E	356	Total	C	N	O	S	Se	0	0	0
			2792	1763	491	524	1	13			
1	F	392	Total	C	N	O	S	Se	0	0	0
			3092	1951	547	578	1	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	initiating methionine	UNP P0AG32
A	-1	GLY	-	expression tag	UNP P0AG32
A	0	HIS	-	expression tag	UNP P0AG32
A	1	MSE	-	expression tag	UNP P0AG32
B	-2	MSE	-	initiating methionine	UNP P0AG32
B	-1	GLY	-	expression tag	UNP P0AG32
B	0	HIS	-	expression tag	UNP P0AG32
B	1	MSE	-	expression tag	UNP P0AG32
C	-2	MSE	-	initiating methionine	UNP P0AG32
C	-1	GLY	-	expression tag	UNP P0AG32
C	0	HIS	-	expression tag	UNP P0AG32
C	1	MSE	-	expression tag	UNP P0AG32
D	-2	MSE	-	initiating methionine	UNP P0AG32
D	-1	GLY	-	expression tag	UNP P0AG32
D	0	HIS	-	expression tag	UNP P0AG32
D	1	MSE	-	expression tag	UNP P0AG32
E	-2	MSE	-	initiating methionine	UNP P0AG32

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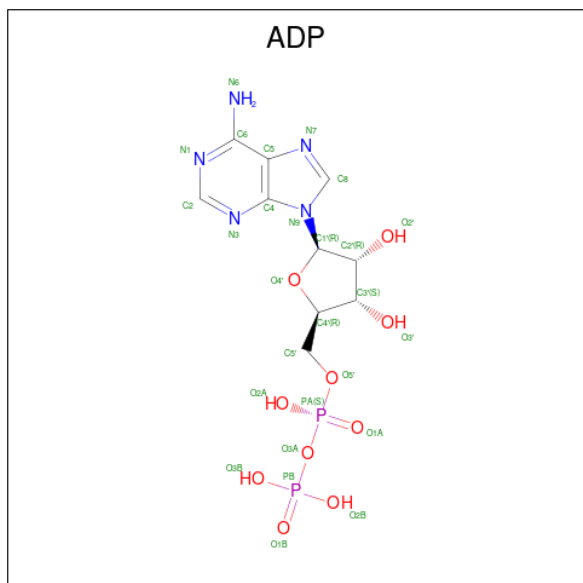
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P0AG32
E	0	HIS	-	expression tag	UNP P0AG32
E	1	MSE	-	expression tag	UNP P0AG32
F	-2	MSE	-	initiating methionine	UNP P0AG32
F	-1	GLY	-	expression tag	UNP P0AG32
F	0	HIS	-	expression tag	UNP P0AG32
F	1	MSE	-	expression tag	UNP P0AG32

- Molecule 2 is a RNA chain called rA12: RNA (5'-R(P*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	P	0	0	0
			155	70	35	43	7			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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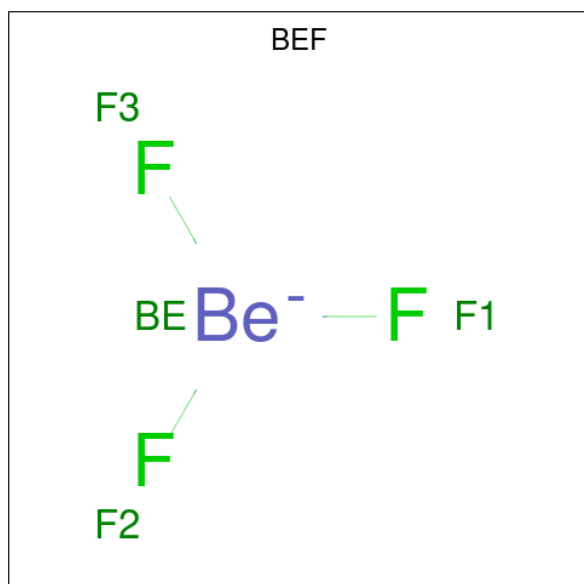
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	Be 1	F 3	0	0
5	C	1	Total 4	Be 1	F 3	0	0
5	D	1	Total 4	Be 1	F 3	0	0
5	E	1	Total 4	Be 1	F 3	0	0
5	F	1	Total 4	Be 1	F 3	0	0

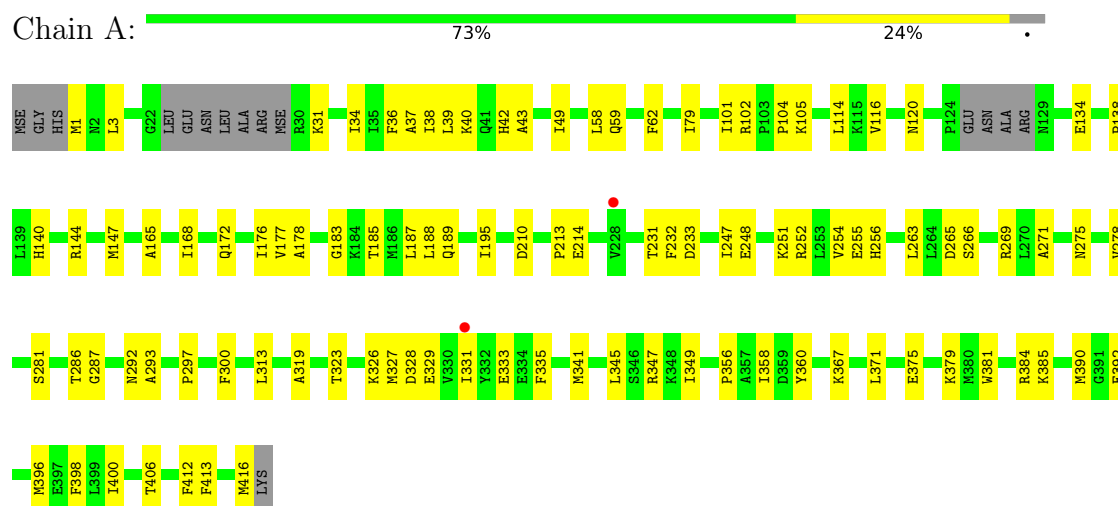
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	3	Total 3	O 3	0	0
6	C	3	Total 3	O 3	0	0
6	D	3	Total 3	O 3	0	0
6	E	3	Total 3	O 3	0	0
6	F	3	Total 3	O 3	0	0
6	G	1	Total 1	O 1	0	0

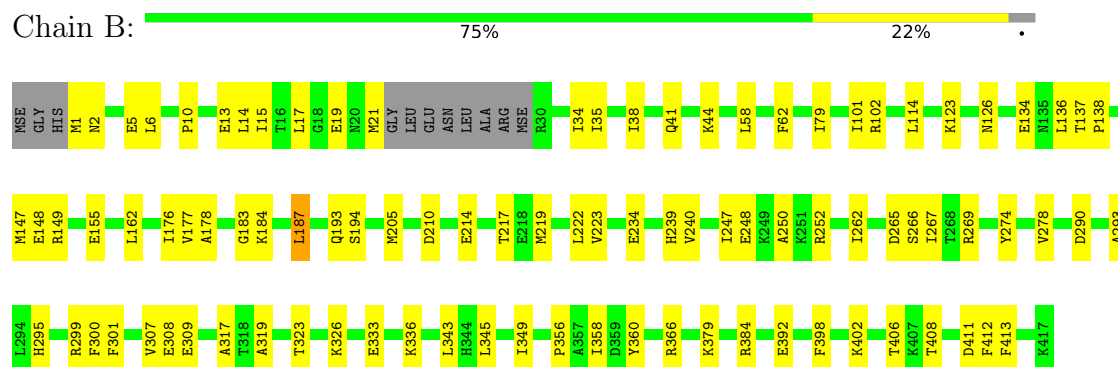
3 Residue-property plots

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.

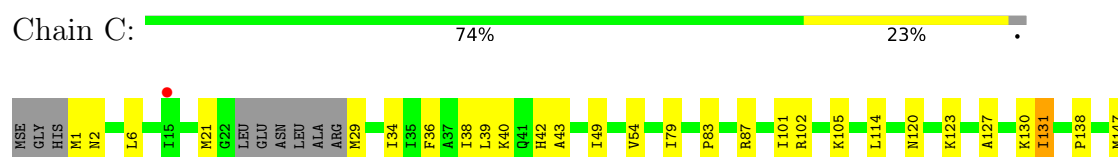
• Molecule 1: Transcription termination factor Rho

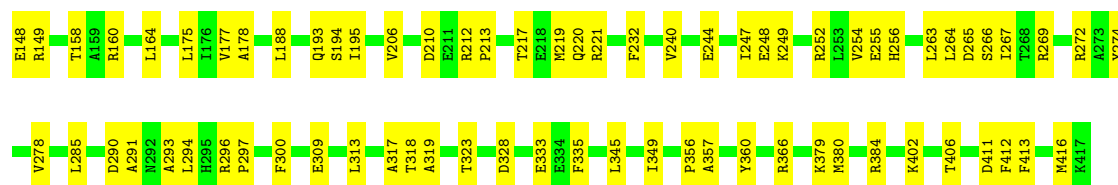


• Molecule 1: Transcription termination factor Rho

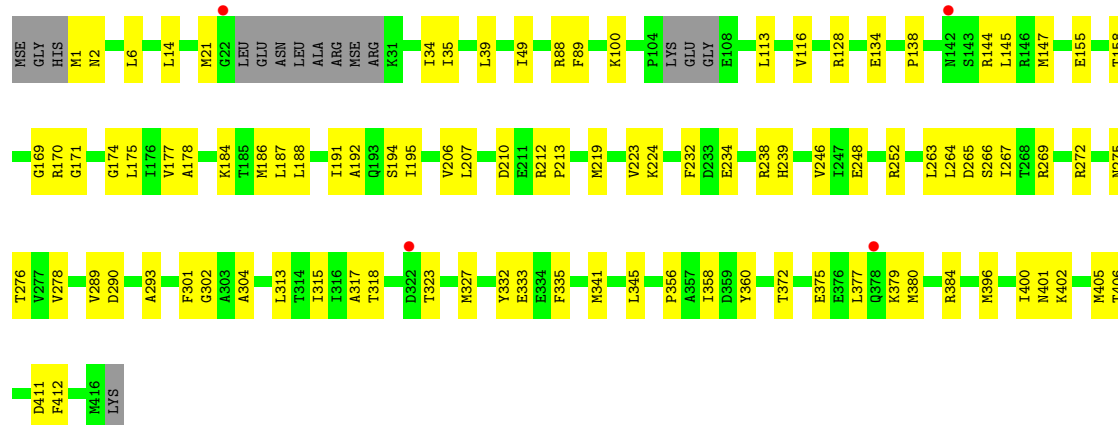


• Molecule 1: Transcription termination factor Rho

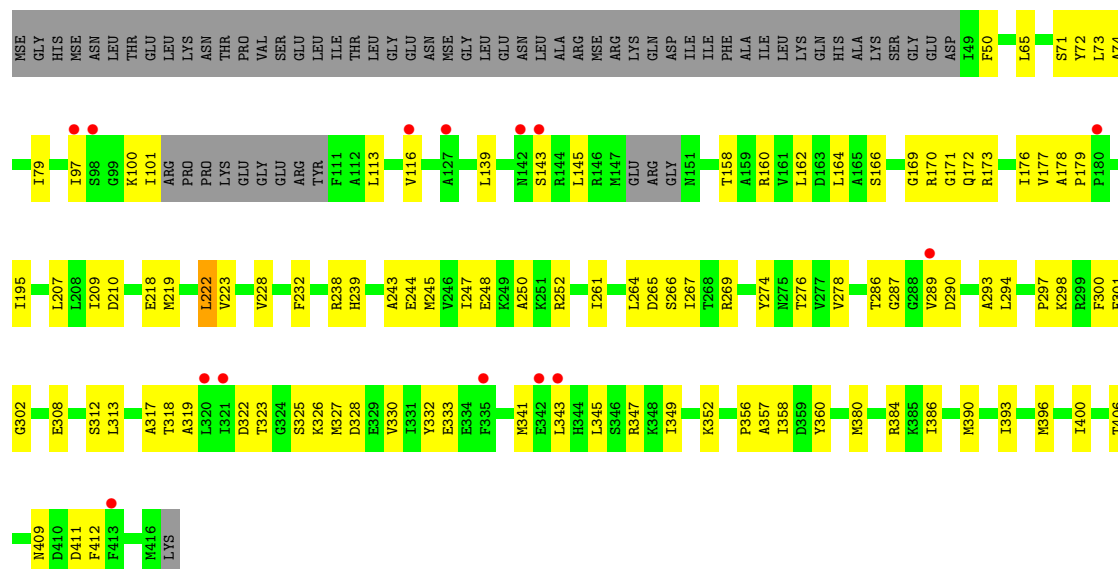




• Molecule 1: Transcription termination factor Rho

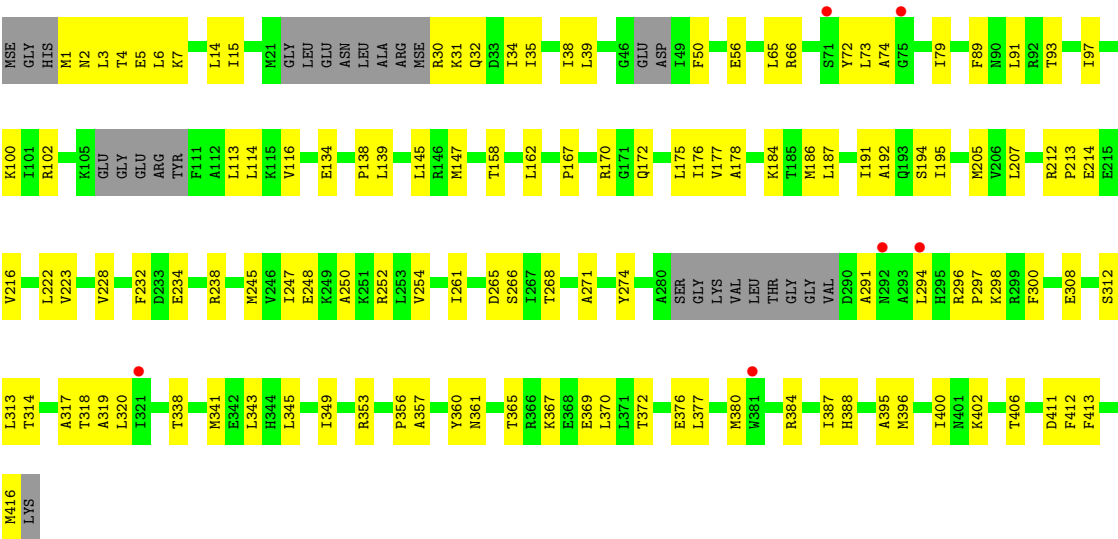


• Molecule 1: Transcription termination factor Rho

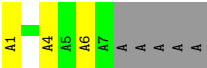
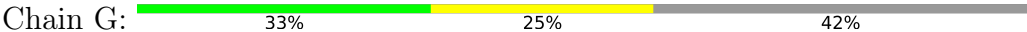


• Molecule 1: Transcription termination factor Rho





● Molecule 2: rA12: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.76Å 199.21Å 112.20Å 90.00° 104.83° 90.00°	Depositor
Resolution (Å)	49.80 – 3.15 49.80 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.80-3.15) 98.8 (49.80-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.233 , 0.265 0.235 , 0.266	Depositor DCC
R_{free} test set	2517 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19062	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BEF, 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	0.12	0/3214	0.32	0/4304
1	B	0.12	0/3253	0.32	0/4357
1	C	0.13	0/3265	0.31	0/4372
1	D	0.13	0/3214	0.31	0/4306
1	E	0.13	0/2820	0.32	0/3778
1	F	0.13	0/3122	0.32	0/4178
2	G	0.46	1/175 (0.6%)	0.14	0/269
All	All	0.13	1/19063 (0.0%)	0.31	0/25564

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	A	OP3-P	6.00	1.60	1.48

There are no bond angle outliers.

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	3181	0	3252	68	0
1	B	3219	0	3293	61	0
1	C	3231	0	3305	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3181	0	3247	67	0
1	E	2792	0	2850	75	0
1	F	3092	0	3167	82	0
2	G	155	0	78	2	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
6	E	3	0	0	0	0
6	F	3	0	0	0	0
6	G	1	0	0	1	0
All	All	19062	0	19264	407	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 (407) 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:A:323:THR:HA	1:B:333:GLU:HG2	1.62	0.82
1:E:177:VAL:HG12	1:E:319:ALA:HB3	1.63	0.80
1:A:1:MSE:HE3	1:A:39:LEU:HD23	1.64	0.77
1:A:1:MSE:HE1	1:A:38:ILE:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:GLN:HE21	1:E:341:MSE:HB2	1.49	0.76
1:A:210:ASP:HB3	1:A:269:ARG:HB3	1.68	0.76
1:C:147:MSE:HE3	1:C:194:SER:HB2	1.66	0.75
1:B:323:THR:HA	1:C:333:GLU:HG2	1.69	0.73
1:E:210:ASP:HB3	1:E:269:ARG:HD3	1.71	0.73
1:F:6:LEU:HD23	1:F:35:ILE:HG13	1.71	0.72
1:E:162:LEU:HD13	1:E:343:LEU:HD22	1.72	0.72
1:D:406:THR:HG21	1:D:411:ASP:HB2	1.72	0.71
1:E:323:THR:HG23	1:E:325:SER:H	1.58	0.69
1:C:323:THR:HA	1:D:333:GLU:HG2	1.74	0.68
1:F:73:LEU:HD11	1:F:238:ARG:HG3	1.75	0.68
1:B:6:LEU:HD23	1:B:35:ILE:HG23	1.77	0.66
1:A:43:ALA:HB2	1:A:49:ILE:HD11	1.78	0.66
1:E:360:TYR:HE2	1:E:384:ARG:HG2	1.60	0.66
1:B:210:ASP:HB3	1:B:269:ARG:HB3	1.76	0.66
1:C:188:LEU:HD11	1:C:263:LEU:HB3	1.78	0.66
1:F:369:GLU:HG2	1:F:370:LEU:HD12	1.78	0.66
1:F:113:LEU:HD21	1:F:116:VAL:HG12	1.77	0.65
1:F:234:GLU:HB3	1:F:238:ARG:HD3	1.78	0.65
1:C:290:ASP:HB3	1:C:293:ALA:HB2	1.79	0.65
1:A:278:VAL:HG21	1:A:293:ALA:HB2	1.79	0.65
1:F:147:MSE:HE3	1:F:194:SER:HB2	1.79	0.64
1:A:79:ILE:HD13	1:A:101:ILE:HG21	1.79	0.64
1:F:4:THR:HA	1:F:7:LYS:HE2	1.79	0.64
1:C:1:MSE:HE3	1:C:39:LEU:HD23	1.79	0.64
1:C:147:MSE:HE1	1:C:195:ILE:HG13	1.80	0.63
1:E:79:ILE:HD13	1:E:101:ILE:HG21	1.80	0.63
1:E:158:THR:HA	1:E:356:PRO:HG3	1.80	0.63
1:F:176:ILE:HB	1:F:318:THR:HG22	1.81	0.63
1:A:375:GLU:HG2	1:A:379:LYS:HE3	1.81	0.62
1:F:192:ALA:HB1	1:F:223:VAL:HG21	1.81	0.62
1:C:79:ILE:HD13	1:C:101:ILE:HG21	1.82	0.62
1:D:192:ALA:HB1	1:D:223:VAL:HG23	1.81	0.62
1:F:177:VAL:HG22	1:F:319:ALA:HB3	1.81	0.62
2:G:4:A:N6	6:G:101:HOH:O	2.30	0.61
1:F:72:TYR:HB3	1:F:245:MSE:HG2	1.82	0.61
1:F:367:LYS:HB3	1:F:370:LEU:HD13	1.82	0.61
1:C:120:ASN:HD22	1:C:256:HIS:CE1	2.17	0.61
1:C:1:MSE:HE1	1:C:38:ILE:HG22	1.83	0.60
1:B:162:LEU:HD13	1:B:343:LEU:HD22	1.82	0.60
1:B:217:THR:HG21	1:C:138:PRO:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:MSE:HG3	3:F:1000:ADP:C8	2.37	0.60
1:A:286:THR:HG22	1:A:326:LYS:HG2	1.84	0.59
1:B:147:MSE:HE3	1:B:194:SER:HB2	1.83	0.59
1:E:173:ARG:HG2	1:E:301:PHE:CZ	2.37	0.59
1:C:267:ILE:HB	1:C:317:ALA:HB1	1.85	0.59
1:E:276:THR:HG23	1:F:291:ALA:HB3	1.83	0.59
1:E:50:PHE:HA	1:E:100:LYS:HA	1.85	0.59
1:A:213:PRO:HB2	1:B:138:PRO:HG2	1.84	0.58
1:B:102:ARG:HB2	1:B:114:LEU:HD11	1.85	0.58
1:F:213:PRO:HD3	1:F:232:PHE:CE2	2.38	0.58
1:F:271:ALA:HB1	1:F:294:LEU:HD22	1.84	0.58
1:A:347:ARG:HH21	1:B:336:LYS:HD3	1.67	0.58
1:B:379:LYS:HD2	1:B:413:PHE:HB3	1.84	0.58
1:D:372:THR:HG21	1:D:380:MSE:HE1	1.84	0.58
1:C:360:TYR:HE2	1:C:384:ARG:HG2	1.68	0.58
1:D:1:MSE:HB3	1:D:49:ILE:HD12	1.85	0.58
1:D:145:LEU:HD11	1:D:170:ARG:HG2	1.85	0.58
1:C:206:VAL:HG11	1:C:219:MSE:HG2	1.84	0.57
1:F:377:LEU:HA	1:F:380:MSE:HE2	1.86	0.57
1:A:172:GLN:HE21	1:A:341:MSE:HB2	1.68	0.57
1:A:356:PRO:HD2	1:A:400:ILE:HD11	1.86	0.57
1:C:210:ASP:HB3	1:C:269:ARG:HB3	1.85	0.57
1:C:175:LEU:HD11	1:C:335:PHE:HB3	1.85	0.57
1:A:177:VAL:HG22	1:A:319:ALA:HB3	1.86	0.57
1:F:102:ARG:HG2	1:F:114:LEU:HD11	1.86	0.57
1:E:176:ILE:HB	1:E:318:THR:HG22	1.86	0.57
1:E:178:ALA:HB2	1:E:345:LEU:HB2	1.86	0.57
1:F:341:MSE:HG2	1:F:365:THR:HG22	1.86	0.56
1:A:406:THR:HG21	1:A:412:PHE:N	2.21	0.56
1:D:206:VAL:HG11	1:D:219:MSE:HG2	1.88	0.56
1:F:172:GLN:HE21	1:F:341:MSE:HB2	1.70	0.56
1:C:43:ALA:HB2	1:C:49:ILE:HD11	1.88	0.56
1:C:217:THR:HG21	1:D:138:PRO:O	2.04	0.56
1:D:402:LYS:HB3	1:D:412:PHE:HE1	1.70	0.56
1:D:396:MSE:HA	1:D:396:MSE:HE2	1.88	0.56
1:A:213:PRO:HD3	1:A:232:PHE:CE2	2.41	0.56
1:A:36:PHE:HE1	1:A:104:PRO:HD2	1.71	0.55
1:D:323:THR:HA	1:E:333:GLU:HG2	1.88	0.55
1:D:356:PRO:HB2	1:D:358:ILE:HG13	1.88	0.55
1:E:145:LEU:HD21	1:E:170:ARG:HG2	1.88	0.55
1:A:120:ASN:HD22	1:A:256:HIS:CE1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HG2	1:A:42:HIS:CD2	2.41	0.55
1:A:147:MSE:HE3	1:A:168:ILE:HD12	1.87	0.54
1:E:158:THR:HG22	1:E:356:PRO:HB3	1.89	0.54
1:D:178:ALA:HB2	1:D:345:LEU:HB2	1.89	0.54
1:A:247:ILE:HB	1:A:300:PHE:CE1	2.42	0.54
1:A:379:LYS:NZ	1:A:413:PHE:HB3	2.23	0.54
1:C:158:THR:HA	1:C:356:PRO:HG3	1.88	0.54
1:E:232:PHE:CE1	1:F:338:THR:HG23	2.42	0.54
1:D:89:PHE:HA	1:D:128:ARG:HD3	1.88	0.54
1:F:387:ILE:HG23	1:F:395:ALA:HB1	1.90	0.54
1:A:39:LEU:HD22	1:A:49:ILE:HG23	1.89	0.54
1:B:21:MSE:SE	1:B:38:ILE:HG23	2.57	0.54
1:F:6:LEU:HG	1:F:14:LEU:HD11	1.89	0.54
1:A:349:ILE:HD11	1:A:392:GLU:HB2	1.90	0.54
1:C:266:SER:HB3	1:C:269:ARG:HG2	1.90	0.54
1:A:102:ARG:HG2	1:A:114:LEU:HD11	1.90	0.53
1:A:231:THR:HG22	1:A:233:ASP:H	1.73	0.53
1:A:254:VAL:HG21	1:A:313:LEU:HB2	1.91	0.53
1:B:219:MSE:O	1:B:223:VAL:HG12	2.09	0.53
1:D:207:LEU:HD13	1:D:246:VAL:HG21	1.91	0.53
1:F:413:PHE:HA	1:F:416:MSE:HE2	1.90	0.53
1:F:205:MSE:HE1	1:F:250:ALA:HB2	1.89	0.53
1:C:102:ARG:HB3	1:C:114:LEU:HD21	1.91	0.53
1:D:210:ASP:HB3	1:D:269:ARG:HB3	1.91	0.53
1:C:213:PRO:HD3	1:C:232:PHE:CE2	2.44	0.53
1:F:294:LEU:C	1:F:297:PRO:HD2	2.34	0.53
1:B:102:ARG:CB	1:B:114:LEU:HD11	2.39	0.53
1:B:247:ILE:HB	1:B:300:PHE:CE1	2.43	0.53
1:C:402:LYS:HB3	1:C:412:PHE:HE1	1.75	0.52
1:F:167:PRO:O	1:F:365:THR:HG21	2.09	0.52
1:E:274:TYR:CD2	1:E:297:PRO:HG3	2.44	0.52
1:A:281:SER:HB3	1:A:292:ASN:ND2	2.24	0.52
1:A:329:GLU:O	1:A:333:GLU:HG2	2.09	0.52
1:F:158:THR:HA	1:F:356:PRO:HG3	1.91	0.52
1:D:219:MSE:O	1:D:223:VAL:HG12	2.09	0.52
1:A:188:LEU:HD11	1:A:263:LEU:HB3	1.92	0.52
1:D:14:LEU:HD12	1:D:34:ILE:HD12	1.92	0.52
1:E:244:GLU:HA	1:E:247:ILE:HG22	1.92	0.52
1:E:267:ILE:HB	1:E:317:ALA:HB1	1.92	0.51
1:B:178:ALA:HB2	1:B:345:LEU:HB2	1.93	0.51
1:B:149:ARG:HH21	1:B:193:GLN:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:PRO:HG2	1:E:347:ARG:HB2	1.91	0.51
1:F:102:ARG:CG	1:F:114:LEU:HD11	2.40	0.51
1:B:79:ILE:HD13	1:B:101:ILE:HG21	1.92	0.51
1:F:139:LEU:CD2	1:F:308:GLU:HB2	2.41	0.51
1:F:178:ALA:HB2	1:F:345:LEU:HB2	1.92	0.51
1:E:289:VAL:HG22	1:E:327:MSE:HG3	1.93	0.51
1:C:217:THR:O	1:C:221:ARG:HD3	2.11	0.51
1:C:267:ILE:HG22	1:C:318:THR:O	2.10	0.51
1:E:113:LEU:HD11	1:E:116:VAL:HG13	1.92	0.51
1:B:15:ILE:O	1:B:19:GLU:HG2	2.10	0.51
1:A:275:ASN:ND2	1:A:327:MSE:HE1	2.25	0.50
1:D:360:TYR:HE2	1:D:384:ARG:HD2	1.76	0.50
1:C:379:LYS:HD3	1:C:413:PHE:HB3	1.93	0.50
1:E:178:ALA:CB	1:E:345:LEU:HB2	2.41	0.50
1:F:247:ILE:HB	1:F:300:PHE:CE1	2.46	0.50
1:E:73:LEU:HD22	1:E:74:ALA:H	1.75	0.50
1:F:3:LEU:HD12	1:F:35:ILE:HD11	1.92	0.50
1:B:234:GLU:HB2	1:B:239:HIS:HE1	1.75	0.50
1:B:406:THR:CG2	1:B:411:ASP:HB2	2.41	0.50
1:E:290:ASP:HB3	1:E:293:ALA:HB2	1.93	0.50
1:B:266:SER:HB3	1:B:269:ARG:HG2	1.93	0.50
1:B:1:MSE:HE2	1:B:6:LEU:HD22	1.93	0.50
1:A:3:LEU:HD23	1:A:39:LEU:HD11	1.94	0.49
1:C:212:ARG:HA	1:C:232:PHE:HE2	1.77	0.49
1:E:278:VAL:HG11	1:E:293:ALA:HB2	1.94	0.49
1:A:356:PRO:HB2	1:A:358:ILE:HG13	1.93	0.49
1:B:58:LEU:HD12	1:B:62:PHE:CE1	2.47	0.49
1:C:149:ARG:HH21	1:C:193:GLN:HB3	1.77	0.49
1:C:178:ALA:HB2	1:C:345:LEU:HB2	1.93	0.49
1:E:172:GLN:NE2	1:E:341:MSE:HB2	2.25	0.49
1:E:177:VAL:HG11	1:E:332:TYR:CD1	2.48	0.49
1:F:360:TYR:CE2	1:F:384:ARG:HG2	2.47	0.49
1:A:327:MSE:HG3	1:A:328:ASP:N	2.27	0.49
1:E:323:THR:HG21	1:E:328:ASP:OD2	2.12	0.49
1:E:356:PRO:HB2	1:E:358:ILE:HG13	1.92	0.49
1:F:207:LEU:HA	1:F:228:VAL:O	2.13	0.49
1:F:248:GLU:O	1:F:252:ARG:HG2	2.13	0.49
1:F:2:ASN:HB3	1:F:5:GLU:HB3	1.94	0.49
1:F:50:PHE:CE1	1:F:100:LYS:HG2	2.48	0.49
1:E:195:ILE:HD13	1:E:261:ILE:HG21	1.94	0.49
1:E:349:ILE:HB	1:E:357:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:O	1:C:252:ARG:HG2	2.13	0.49
1:E:406:THR:HG21	1:E:412:PHE:N	2.28	0.49
1:F:139:LEU:HD23	1:F:308:GLU:HB2	1.94	0.49
3:A:1000:ADP:O1A	1:B:366:ARG:NH2	2.46	0.48
1:F:138:PRO:C	1:F:139:LEU:HD22	2.38	0.48
1:C:127:ALA:O	1:C:130:LYS:HD2	2.14	0.48
1:D:272:ARG:O	1:D:276:THR:HG23	2.13	0.48
1:E:218:GLU:O	1:E:222:LEU:HD12	2.13	0.48
1:B:406:THR:HG22	1:B:408:THR:H	1.79	0.48
1:C:83:PRO:O	1:C:87:ARG:HG3	2.13	0.48
1:F:89:PHE:HB2	1:F:91:LEU:HG	1.96	0.48
1:F:178:ALA:CB	1:F:345:LEU:HB2	2.43	0.48
1:A:102:ARG:NH1	1:A:105:LYS:HG3	2.28	0.48
1:E:171:GLY:HA2	1:E:313:LEU:O	2.14	0.48
1:B:278:VAL:HG11	1:B:293:ALA:HB2	1.95	0.48
1:B:148:GLU:OE1	1:B:408:THR:HA	2.14	0.48
1:D:88:ARG:O	1:D:128:ARG:HD3	2.14	0.48
1:C:232:PHE:CE1	1:D:302:GLY:HA3	2.49	0.48
1:D:147:MSE:HE3	1:D:194:SER:HB2	1.96	0.47
1:F:294:LEU:O	1:F:298:LYS:HG3	2.14	0.47
1:A:178:ALA:HB2	1:A:345:LEU:HB2	1.96	0.47
1:F:1:MSE:HE3	1:F:39:LEU:HD23	1.96	0.47
1:C:294:LEU:C	1:C:297:PRO:HD2	2.39	0.47
1:A:134:GLU:CD	1:A:134:GLU:H	2.22	0.47
1:D:401:ASN:O	1:D:405:MSE:HG3	2.14	0.47
1:F:147:MSE:HG3	1:F:162:LEU:HD22	1.97	0.47
1:C:360:TYR:CE2	1:C:384:ARG:HG2	2.49	0.47
1:E:164:LEU:HD23	1:E:380:MSE:HE2	1.96	0.47
1:D:275:ASN:HA	1:D:293:ALA:HB1	1.97	0.47
1:D:278:VAL:HG11	1:D:293:ALA:HA	1.97	0.47
1:F:1:MSE:HE1	1:F:38:ILE:HG22	1.96	0.47
1:A:37:ALA:HA	1:A:40:LYS:HE2	1.95	0.47
1:E:209:ILE:HG23	1:E:239:HIS:HB3	1.96	0.47
1:A:176:ILE:HD13	1:A:187:LEU:HD12	1.96	0.47
1:C:177:VAL:HG22	1:C:319:ALA:HB3	1.97	0.47
1:D:234:GLU:HB2	1:D:239:HIS:CE1	2.50	0.47
1:F:265:ASP:HA	1:F:266:SER:HA	1.60	0.47
1:C:265:ASP:HA	1:C:266:SER:HA	1.54	0.46
1:F:2:ASN:O	1:F:6:LEU:HB2	2.15	0.46
1:E:177:VAL:HG11	1:E:332:TYR:CE1	2.50	0.46
1:A:271:ALA:HB1	1:A:331:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:MSE:HE1	3:D:1000:ADP:H3'	1.97	0.46
1:D:267:ILE:HD11	1:D:301:PHE:HB2	1.97	0.46
1:D:175:LEU:HD11	1:D:335:PHE:HB3	1.97	0.46
1:D:234:GLU:HB2	1:D:239:HIS:HE1	1.80	0.46
1:D:377:LEU:HA	1:D:380:MSE:HE2	1.98	0.46
1:F:100:LYS:O	1:F:113:LEU:HD12	2.15	0.46
1:F:175:LEU:HA	1:F:317:ALA:O	2.16	0.46
1:A:165:ALA:HA	1:A:384:ARG:HH12	1.81	0.46
1:A:297:PRO:HB2	1:A:335:PHE:CZ	2.50	0.46
1:B:10:PRO:HG2	1:B:13:GLU:HG2	1.96	0.46
1:B:177:VAL:HG22	1:B:319:ALA:HB3	1.97	0.46
1:C:247:ILE:HB	1:C:300:PHE:CE1	2.51	0.46
1:D:212:ARG:HA	1:D:232:PHE:CE2	2.51	0.46
1:D:234:GLU:HB3	1:D:238:ARG:HD3	1.96	0.46
1:D:178:ALA:HB3	1:D:184:LYS:CG	2.46	0.46
1:D:264:LEU:HB3	1:D:317:ALA:HB2	1.97	0.46
1:E:65:LEU:HD21	1:E:97:ILE:HD12	1.96	0.46
1:B:356:PRO:HB2	1:B:358:ILE:HG13	1.97	0.46
1:C:274:TYR:CD2	1:C:297:PRO:HG3	2.51	0.46
1:B:17:LEU:HD21	1:B:21:MSE:HE3	1.97	0.46
1:D:290:ASP:HB3	1:D:293:ALA:HB2	1.98	0.46
1:E:209:ILE:HG12	1:E:264:LEU:HD11	1.98	0.46
1:D:187:LEU:O	1:D:191:ILE:HG12	2.15	0.46
1:D:267:ILE:HB	1:D:317:ALA:HB1	1.98	0.46
1:F:31:LYS:O	1:F:35:ILE:HG22	2.16	0.46
1:B:267:ILE:HB	1:B:317:ALA:HB1	1.98	0.45
1:E:286:THR:O	1:E:330:VAL:HG21	2.16	0.45
1:E:406:THR:HG23	1:E:411:ASP:HB2	1.98	0.45
1:F:254:VAL:HG21	1:F:313:LEU:HB2	1.97	0.45
1:E:219:MSE:O	1:E:223:VAL:HG12	2.16	0.45
1:E:287:GLY:HA2	1:E:326:LYS:HB3	1.99	0.45
1:F:145:LEU:HD11	1:F:170:ARG:HG3	1.99	0.45
1:B:360:TYR:CE2	1:B:384:ARG:HD2	2.52	0.45
1:A:360:TYR:HB2	1:A:396:MSE:HE3	1.99	0.45
1:C:36:PHE:CE1	1:C:40:LYS:HD2	2.52	0.45
1:C:102:ARG:NH1	1:C:105:LYS:HG3	2.31	0.45
1:E:71:SER:HB2	1:E:238:ARG:NH2	2.31	0.45
1:F:65:LEU:HD21	1:F:97:ILE:HD12	1.98	0.45
1:A:168:ILE:HD11	1:A:341:MSE:HE3	1.99	0.45
1:A:233:ASP:HB3	1:B:299:ARG:HH11	1.82	0.45
1:C:130:LYS:HE2	1:C:255:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:VAL:HG11	1:C:293:ALA:HB2	1.99	0.45
1:E:179:PRO:HG3	1:E:322:ASP:HB2	1.99	0.45
1:F:56:GLU:HA	1:F:93:THR:HG23	1.98	0.45
1:F:134:GLU:H	1:F:134:GLU:CD	2.25	0.45
1:D:134:GLU:H	1:D:134:GLU:CD	2.25	0.45
1:E:72:TYR:HB3	1:E:245:MSE:HE2	1.99	0.45
1:E:352:LYS:HD3	1:E:393:ILE:HG21	1.98	0.45
1:B:295:HIS:CE1	1:B:299:ARG:HD2	2.52	0.45
1:D:155:GLU:H	1:D:155:GLU:CD	2.25	0.45
1:D:356:PRO:HD2	1:D:400:ILE:HD11	1.97	0.45
1:A:147:MSE:HE1	1:A:195:ILE:HD11	1.98	0.44
1:A:248:GLU:O	1:A:252:ARG:HG2	2.17	0.44
1:E:170:ARG:HB3	1:E:312:SER:OG	2.18	0.44
1:D:265:ASP:HA	1:D:266:SER:HA	1.53	0.44
1:A:144:ARG:HD3	1:A:371:LEU:HB3	1.99	0.44
1:D:406:THR:CG2	1:D:411:ASP:HB2	2.44	0.44
1:B:134:GLU:CD	1:B:134:GLU:H	2.26	0.44
1:E:266:SER:HB2	1:E:318:THR:O	2.17	0.44
1:B:248:GLU:O	1:B:252:ARG:HG2	2.18	0.44
1:C:175:LEU:HA	1:C:317:ALA:O	2.17	0.44
1:E:386:ILE:HG22	1:E:390:MSE:HE3	1.99	0.44
1:F:268:THR:HG21	1:F:320:LEU:H	1.81	0.44
1:A:31:LYS:HA	1:A:34:ILE:HG22	1.99	0.44
1:A:381:TRP:O	1:A:385:LYS:HG3	2.16	0.44
1:B:123:LYS:HB2	1:B:126:ASN:HD22	1.81	0.44
1:C:272:ARG:HH21	1:C:328:ASP:CG	2.26	0.44
1:C:296:ARG:HB2	1:C:297:PRO:HD3	1.98	0.44
1:D:100:LYS:O	1:D:113:LEU:HD22	2.18	0.44
1:E:173:ARG:HD2	1:E:302:GLY:HA2	2.00	0.44
1:F:212:ARG:HB3	1:F:214:GLU:OE1	2.18	0.44
1:A:271:ALA:HB1	1:A:331:ILE:HG21	2.00	0.44
1:C:178:ALA:CB	1:C:345:LEU:HB2	2.48	0.44
1:C:349:ILE:HB	1:C:357:ALA:HB1	2.00	0.43
1:D:191:ILE:O	1:D:195:ILE:HG12	2.17	0.43
1:A:265:ASP:HA	1:A:266:SER:HA	1.57	0.43
1:B:326:LYS:NZ	2:G:6:A:H61	2.16	0.43
1:D:1:MSE:HE3	1:D:21:MSE:HE1	1.98	0.43
1:E:207:LEU:O	1:E:264:LEU:HA	2.18	0.43
1:A:178:ALA:CB	1:A:345:LEU:HB2	2.48	0.43
1:F:361:ASN:OD1	1:F:388:HIS:HA	2.18	0.43
1:A:412:PHE:CE2	1:A:416:MSE:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ALA:CB	1:D:345:LEU:HB2	2.48	0.43
1:C:267:ILE:HG13	1:C:335:PHE:CE1	2.54	0.43
1:D:232:PHE:CE1	1:E:302:GLY:HA3	2.54	0.43
1:D:213:PRO:HD3	1:D:232:PHE:CZ	2.53	0.43
1:D:375:GLU:O	1:D:379:LYS:HG2	2.18	0.43
1:F:170:ARG:HB3	1:F:312:SER:OG	2.19	0.43
1:F:261:ILE:HG12	1:F:314:THR:HB	2.01	0.43
1:C:285:LEU:HD13	1:C:291:ALA:HA	1.99	0.43
1:D:304:ALA:HB2	1:D:315:ILE:HG13	2.01	0.43
1:D:380:MSE:O	1:D:384:ARG:HB2	2.19	0.43
1:E:139:LEU:HD12	1:E:308:GLU:HB3	2.00	0.43
1:F:30:ARG:O	1:F:34:ILE:HG13	2.19	0.43
1:A:172:GLN:NE2	1:A:341:MSE:HB2	2.31	0.43
1:B:178:ALA:CB	1:B:345:LEU:HB2	2.49	0.43
1:A:384:ARG:HG2	1:F:353:ARG:HG2	2.00	0.43
1:C:212:ARG:HA	1:C:232:PHE:CE2	2.53	0.43
1:C:240:VAL:O	1:C:244:GLU:HG2	2.19	0.43
1:E:250:ALA:HB1	1:E:313:LEU:HD13	2.01	0.43
1:A:138:PRO:HG3	1:F:213:PRO:HB2	2.01	0.42
1:A:396:MSE:HE2	1:A:396:MSE:HA	2.01	0.42
1:B:2:ASN:HB3	1:B:5:GLU:HG2	2.00	0.42
1:B:398:PHE:O	1:B:402:LYS:HG2	2.19	0.42
1:C:2:ASN:O	1:C:6:LEU:HD13	2.19	0.42
1:E:143:SER:HB3	1:E:170:ARG:HG3	2.01	0.42
1:E:265:ASP:HA	1:E:266:SER:HA	1.55	0.42
1:B:136:LEU:HB3	1:B:307:VAL:HG13	2.01	0.42
1:C:131:ILE:HD12	1:C:309:GLU:HG2	2.00	0.42
1:C:148:GLU:HG3	1:C:160:ARG:HG2	2.01	0.42
1:D:171:GLY:HA2	1:D:313:LEU:O	2.19	0.42
1:E:360:TYR:CE2	1:E:384:ARG:HG2	2.48	0.42
1:F:356:PRO:HD2	1:F:400:ILE:HD11	2.02	0.42
1:A:58:LEU:HD12	1:A:62:PHE:CE1	2.54	0.42
3:B:1000:ADP:O2A	1:C:366:ARG:NH2	2.52	0.42
1:C:29:MSE:HG3	1:C:34:ILE:HD12	2.01	0.42
1:E:207:LEU:HA	1:E:228:VAL:O	2.18	0.42
1:E:294:LEU:O	1:E:298:LYS:HB2	2.19	0.42
1:F:402:LYS:HB3	1:F:412:PHE:HE1	1.84	0.42
1:E:356:PRO:O	1:E:396:MSE:HE2	2.19	0.42
1:F:50:PHE:CD1	1:F:100:LYS:HG2	2.53	0.42
1:F:176:ILE:HD12	1:F:343:LEU:HD23	2.01	0.42
1:B:183:GLY:O	1:B:187:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:HB2	1:B:239:HIS:CE1	2.53	0.42
1:B:290:ASP:HB3	1:B:293:ALA:HB2	2.01	0.42
1:D:35:ILE:O	1:D:39:LEU:HG	2.20	0.42
1:F:296:ARG:HB2	1:F:297:PRO:HD3	2.00	0.42
1:E:345:LEU:HA	1:E:357:ALA:O	2.20	0.42
1:C:54:VAL:HG21	1:C:249:LYS:HD2	2.02	0.42
1:D:224:LYS:HD3	1:D:224:LYS:HA	1.90	0.42
1:E:396:MSE:O	1:E:400:ILE:HG12	2.20	0.42
1:B:265:ASP:HA	1:B:266:SER:HA	1.55	0.42
1:C:21:MSE:SE	1:C:38:ILE:HG23	2.70	0.42
1:E:406:THR:CG2	1:E:411:ASP:HB2	2.50	0.42
1:A:214:GLU:H	1:A:214:GLU:CD	2.27	0.42
1:B:41:GLN:HG3	1:B:44:LYS:HD2	2.01	0.42
1:D:375:GLU:H	1:D:375:GLU:CD	2.27	0.42
1:E:289:VAL:CG2	1:E:327:MSE:HG3	2.50	0.42
1:F:15:ILE:HG12	1:F:34:ILE:HD13	2.02	0.42
1:F:178:ALA:HB3	1:F:184:LYS:CG	2.50	0.41
1:C:379:LYS:HB3	1:C:416:MSE:HE1	2.00	0.41
1:D:267:ILE:HG22	1:D:318:THR:O	2.20	0.41
1:E:247:ILE:HB	1:E:300:PHE:CE1	2.56	0.41
1:F:406:THR:CG2	1:F:411:ASP:HB2	2.51	0.41
1:A:49:ILE:HB	1:A:101:ILE:O	2.20	0.41
1:A:390:MSE:HE1	1:A:398:PHE:HB2	2.01	0.41
1:B:178:ALA:HB3	1:B:184:LYS:CG	2.50	0.41
1:D:6:LEU:HD22	1:D:39:LEU:HD21	2.02	0.41
1:D:144:ARG:HA	1:D:169:GLY:HA2	2.02	0.41
1:D:174:GLY:HA3	1:D:341:MSE:SE	2.70	0.41
1:D:188:LEU:HD11	1:D:263:LEU:HB3	2.03	0.41
1:E:248:GLU:O	1:E:252:ARG:HG2	2.20	0.41
1:C:406:THR:HG21	1:C:412:PHE:HB2	2.02	0.41
1:F:376:GLU:O	1:F:380:MSE:HG3	2.20	0.41
1:F:396:MSE:O	1:F:400:ILE:HG12	2.20	0.41
1:B:205:MSE:HE1	1:B:250:ALA:HB2	2.03	0.41
1:F:3:LEU:HD23	1:F:79:ILE:HD11	2.01	0.41
1:B:349:ILE:HD11	1:B:392:GLU:HB3	2.02	0.41
1:D:289:VAL:CG2	1:D:327:MSE:HG3	2.51	0.41
1:B:137:THR:HG23	1:B:308:GLU:HB3	2.01	0.41
1:B:402:LYS:HB3	1:B:412:PHE:HE1	1.86	0.41
1:C:36:PHE:CZ	1:C:40:LYS:HD2	2.56	0.41
1:D:158:THR:HA	1:D:356:PRO:HG3	2.03	0.41
1:A:287:GLY:HA2	1:A:326:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LEU:O	1:C:380:MSE:HE3	2.20	0.41
1:C:406:THR:OG1	1:C:411:ASP:HB2	2.21	0.41
1:F:32:GLN:H	1:F:32:GLN:CD	2.29	0.41
1:F:274:TYR:CD2	1:F:297:PRO:HG3	2.56	0.41
1:F:349:ILE:HB	1:F:357:ALA:HB1	2.02	0.41
1:F:372:THR:HG21	1:F:380:MSE:HE1	2.03	0.41
1:A:140:HIS:CG	1:A:367:LYS:HG3	2.56	0.41
1:A:271:ALA:CB	1:A:331:ILE:HG21	2.51	0.41
1:B:176:ILE:HD12	1:B:343:LEU:HD23	2.03	0.41
1:C:217:THR:HA	1:C:220:GLN:HG2	2.02	0.41
1:C:254:VAL:HG21	1:C:313:LEU:HB2	2.03	0.41
1:E:166:SER:OG	1:E:341:MSE:HE2	2.21	0.41
1:F:191:ILE:O	1:F:195:ILE:HG12	2.22	0.40
1:B:155:GLU:CD	1:B:155:GLU:H	2.29	0.40
1:B:205:MSE:HE3	1:B:262:ILE:HG12	2.03	0.40
1:C:1:MSE:HG2	1:C:42:HIS:CD2	2.57	0.40
1:E:267:ILE:HG22	1:E:318:THR:O	2.20	0.40
1:E:380:MSE:O	1:E:384:ARG:HG3	2.21	0.40
1:F:66:ARG:NH1	1:F:74:ALA:HA	2.36	0.40
1:A:185:THR:O	1:A:189:GLN:HG3	2.20	0.40
1:A:251:LYS:O	1:A:255:GLU:HG3	2.22	0.40
1:B:137:THR:HG22	1:B:309:GLU:OE2	2.21	0.40
1:E:160:ARG:HB3	1:E:409:ASN:OD1	2.20	0.40
1:E:207:LEU:HD21	1:E:243:ALA:HA	2.02	0.40
1:A:183:GLY:O	1:A:187:LEU:HB2	2.21	0.40
1:B:240:VAL:HG13	1:B:274:TYR:CE1	2.56	0.40
1:C:264:LEU:O	1:C:317:ALA:HA	2.22	0.40
1:F:34:ILE:O	1:F:38:ILE:HG13	2.22	0.40
1:B:14:LEU:HB3	1:B:34:ILE:HG21	2.04	0.40
1:B:267:ILE:HD11	1:B:301:PHE:HB2	2.04	0.40
1:D:2:ASN:O	1:D:6:LEU:HD13	2.21	0.40
1:D:177:VAL:HG21	1:D:332:TYR:HE1	1.85	0.40
1:D:248:GLU:O	1:D:252:ARG:HG2	2.21	0.40
1:E:145:LEU:HD23	1:E:169:GLY:C	2.46	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	399/420 (95%)	391 (98%)	8 (2%)	0	100	100
1	B	405/420 (96%)	393 (97%)	12 (3%)	0	100	100
1	C	407/420 (97%)	397 (98%)	10 (2%)	0	100	100
1	D	399/420 (95%)	385 (96%)	14 (4%)	0	100	100
1	E	350/420 (83%)	342 (98%)	8 (2%)	0	100	100
1	F	382/420 (91%)	375 (98%)	7 (2%)	0	100	100
All	All	2342/2520 (93%)	2283 (98%)	59 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	347/342 (102%)	345 (99%)	2 (1%)	78	81
1	B	351/342 (103%)	348 (99%)	3 (1%)	70	77
1	C	352/342 (103%)	350 (99%)	2 (1%)	78	81
1	D	347/342 (102%)	346 (100%)	1 (0%)	86	85
1	E	304/342 (89%)	303 (100%)	1 (0%)	86	85
1	F	338/342 (99%)	335 (99%)	3 (1%)	70	77
All	All	2039/2052 (99%)	2027 (99%)	12 (1%)	78	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	116	VAL
1	B	187	LEU
1	B	214	GLU
1	B	222	LEU
1	C	123	LYS
1	C	131	ILE
1	D	116	VAL
1	E	222	LEU
1	F	187	LEU
1	F	216	VAL
1	F	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	129	ASN
1	A	172	GLN
1	A	193	GLN
1	A	256	HIS
1	B	20	ASN
1	B	59	GLN
1	B	126	ASN
1	B	140	HIS
1	B	189	GLN
1	B	295	HIS
1	B	388	HIS
1	C	20	ASN
1	C	41	GLN
1	C	42	HIS
1	C	172	GLN
1	C	193	GLN
1	C	241	GLN
1	C	256	HIS
1	C	388	HIS
1	D	32	GLN
1	D	117	ASN
1	D	126	ASN
1	E	59	GLN
1	E	172	GLN

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Mol	Chain	Res	Type
1	E	239	HIS
1	E	378	GLN
1	E	388	HIS
1	F	140	HIS
1	F	172	GLN
1	F	189	GLN
1	F	292	ASN
1	F	295	HIS
1	F	388	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/12 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BEF	A	1002	3	0,3,3	-	-	-		
3	ADP	B	1000	5,4	28,29,29	1.42	4 (14%)	43,45,45	1.88	11 (25%)
3	ADP	D	1000	5,4	28,29,29	1.41	4 (14%)	43,45,45	1.87	10 (23%)
5	BEF	C	1002	3	0,3,3	-	-	-		
5	BEF	B	1002	3	0,3,3	-	-	-		
3	ADP	A	1000	5,4	28,29,29	1.41	4 (14%)	43,45,45	1.88	11 (25%)
3	ADP	E	1000	5,4	28,29,29	1.41	4 (14%)	43,45,45	1.87	10 (23%)
3	ADP	F	1000	5,4	28,29,29	1.41	4 (14%)	43,45,45	1.87	10 (23%)
5	BEF	F	1002	3	0,3,3	-	-	-		
5	BEF	E	1002	3	0,3,3	-	-	-		
3	ADP	C	1000	5,4	28,29,29	1.41	4 (14%)	43,45,45	1.88	11 (25%)
5	BEF	D	1002	3	0,3,3	-	-	-		

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
3	ADP	B	1000	5,4	-	3/16/32/32	0/3/3/3
3	ADP	D	1000	5,4	-	3/16/32/32	0/3/3/3
3	ADP	A	1000	5,4	-	2/16/32/32	0/3/3/3
3	ADP	E	1000	5,4	-	2/16/32/32	0/3/3/3
3	ADP	F	1000	5,4	-	2/16/32/32	0/3/3/3
3	ADP	C	1000	5,4	-	3/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ADP	C5-C4	4.76	1.47	1.39
3	D	1000	ADP	C5-C4	4.75	1.47	1.39
3	C	1000	ADP	C5-C4	4.74	1.47	1.39
3	F	1000	ADP	C5-C4	4.74	1.47	1.39
3	E	1000	ADP	C5-C4	4.71	1.47	1.39
3	B	1000	ADP	C5-C4	4.71	1.47	1.39
3	E	1000	ADP	C5-C6	2.74	1.48	1.41
3	A	1000	ADP	C5-C6	2.72	1.48	1.41
3	B	1000	ADP	C5-C6	2.72	1.48	1.41
3	C	1000	ADP	C5-C6	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	ADP	C5-C6	2.71	1.48	1.41
3	F	1000	ADP	C5-C6	2.69	1.48	1.41
3	B	1000	ADP	C8-N7	2.34	1.36	1.31
3	A	1000	ADP	C8-N7	2.33	1.36	1.31
3	E	1000	ADP	C8-N7	2.33	1.36	1.31
3	D	1000	ADP	C8-N7	2.32	1.36	1.31
3	F	1000	ADP	C8-N7	2.32	1.36	1.31
3	C	1000	ADP	C8-N7	2.31	1.36	1.31
3	A	1000	ADP	C5-N7	-2.25	1.35	1.39
3	E	1000	ADP	C5-N7	-2.25	1.35	1.39
3	B	1000	ADP	C5-N7	-2.24	1.35	1.39
3	F	1000	ADP	C5-N7	-2.23	1.35	1.39
3	C	1000	ADP	C5-N7	-2.21	1.35	1.39
3	D	1000	ADP	C5-N7	-2.20	1.35	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1000	ADP	C5-C4-N3	-5.82	118.71	126.72
3	F	1000	ADP	C5-C4-N3	-5.81	118.72	126.72
3	B	1000	ADP	C5-C4-N3	-5.80	118.73	126.72
3	D	1000	ADP	C5-C4-N3	-5.80	118.73	126.72
3	A	1000	ADP	C5-C4-N3	-5.80	118.73	126.72
3	C	1000	ADP	C5-C4-N3	-5.79	118.74	126.72
3	A	1000	ADP	N3-C4-N9	4.71	135.17	127.17
3	E	1000	ADP	N3-C4-N9	4.71	135.17	127.17
3	F	1000	ADP	N3-C4-N9	4.70	135.16	127.17
3	C	1000	ADP	N3-C4-N9	4.69	135.15	127.17
3	D	1000	ADP	N3-C4-N9	4.68	135.13	127.17
3	B	1000	ADP	N3-C4-N9	4.66	135.09	127.17
3	E	1000	ADP	C2-N3-C4	3.72	120.91	111.83
3	C	1000	ADP	C2-N3-C4	3.71	120.90	111.83
3	A	1000	ADP	C2-N3-C4	3.71	120.89	111.83
3	B	1000	ADP	C2-N3-C4	3.70	120.87	111.83
3	D	1000	ADP	C2-N3-C4	3.70	120.87	111.83
3	F	1000	ADP	C2-N3-C4	3.70	120.86	111.83
3	F	1000	ADP	C4-C5-N7	-3.41	106.68	110.58
3	D	1000	ADP	C4-C5-N7	-3.41	106.69	110.58
3	B	1000	ADP	C4-C5-N7	-3.40	106.69	110.58
3	A	1000	ADP	C4-C5-N7	-3.40	106.69	110.58
3	C	1000	ADP	C4-C5-N7	-3.39	106.70	110.58
3	E	1000	ADP	C4-C5-N7	-3.38	106.71	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1000	ADP	N3-C2-N1	-3.29	123.59	128.58
3	B	1000	ADP	N3-C2-N1	-3.28	123.62	128.58
3	D	1000	ADP	N3-C2-N1	-3.26	123.64	128.58
3	A	1000	ADP	N3-C2-N1	-3.25	123.66	128.58
3	E	1000	ADP	N3-C2-N1	-3.25	123.66	128.58
3	F	1000	ADP	N3-C2-N1	-3.23	123.69	128.58
3	A	1000	ADP	C4-N9-C8	2.81	108.69	105.74
3	C	1000	ADP	C4-N9-C8	2.80	108.68	105.74
3	F	1000	ADP	C4-N9-C8	2.80	108.68	105.74
3	E	1000	ADP	C4-N9-C8	2.79	108.67	105.74
3	D	1000	ADP	C4-N9-C8	2.78	108.66	105.74
3	B	1000	ADP	C4-N9-C8	2.77	108.64	105.74
3	D	1000	ADP	C3'-C2'-C1'	2.59	106.37	101.46
3	E	1000	ADP	C3'-C2'-C1'	2.58	106.35	101.46
3	B	1000	ADP	C3'-C2'-C1'	2.58	106.34	101.46
3	F	1000	ADP	C3'-C2'-C1'	2.58	106.34	101.46
3	C	1000	ADP	C3'-C2'-C1'	2.57	106.32	101.46
3	A	1000	ADP	C3'-C2'-C1'	2.57	106.32	101.46
3	A	1000	ADP	C5-N7-C8	2.55	107.45	103.45
3	B	1000	ADP	C5-N7-C8	2.53	107.42	103.45
3	C	1000	ADP	C5-N7-C8	2.52	107.41	103.45
3	F	1000	ADP	C5-N7-C8	2.51	107.40	103.45
3	D	1000	ADP	C5-N7-C8	2.51	107.39	103.45
3	E	1000	ADP	C5-N7-C8	2.50	107.38	103.45
3	A	1000	ADP	C2'-C1'-N9	-2.26	107.70	113.30
3	F	1000	ADP	C2'-C1'-N9	-2.25	107.71	113.30
3	C	1000	ADP	C2'-C1'-N9	-2.24	107.73	113.30
3	D	1000	ADP	C2'-C1'-N9	-2.24	107.75	113.30
3	E	1000	ADP	C2'-C1'-N9	-2.23	107.77	113.30
3	B	1000	ADP	C2'-C1'-N9	-2.22	107.78	113.30
3	A	1000	ADP	C6-C5-N7	2.09	136.11	132.09
3	D	1000	ADP	C6-C5-N7	2.08	136.09	132.09
3	F	1000	ADP	C6-C5-N7	2.07	136.09	132.09
3	C	1000	ADP	C6-C5-N7	2.07	136.08	132.09
3	B	1000	ADP	C6-C5-N7	2.07	136.08	132.09
3	E	1000	ADP	C6-C5-N7	2.06	136.06	132.09
3	B	1000	ADP	N9-C8-N7	-2.02	111.07	113.94
3	A	1000	ADP	N9-C8-N7	-2.02	111.08	113.94
3	C	1000	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

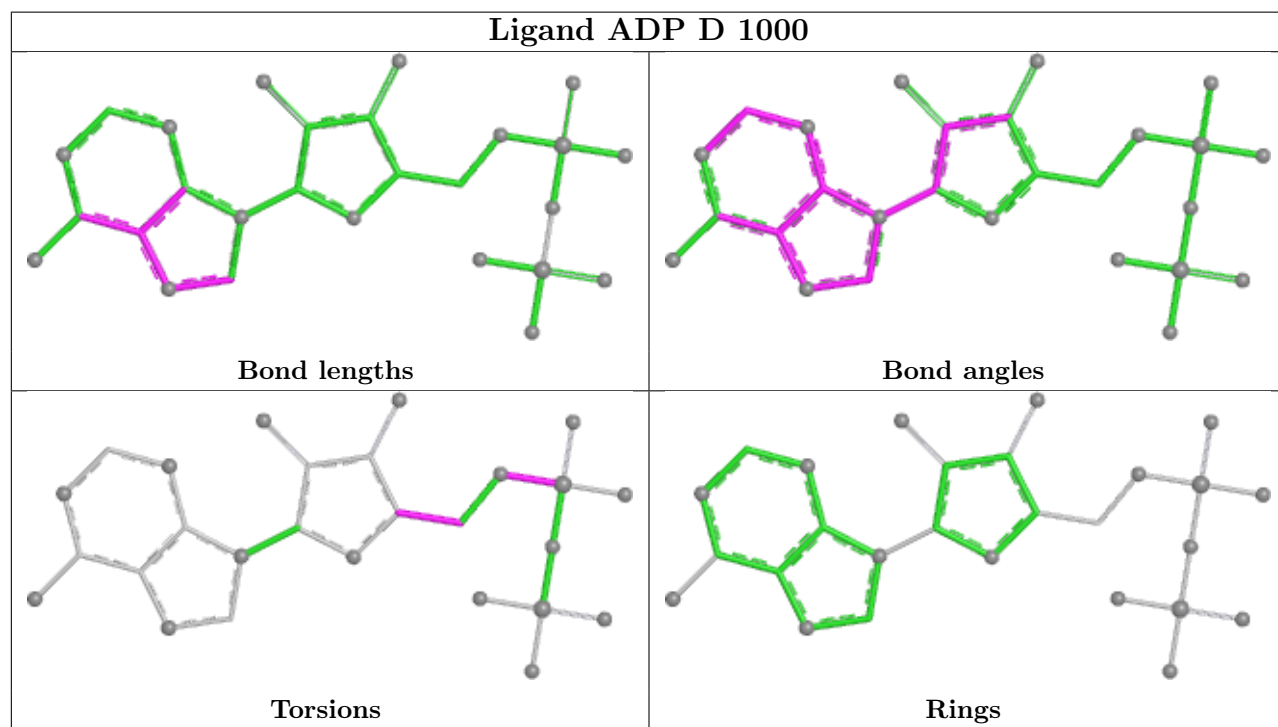
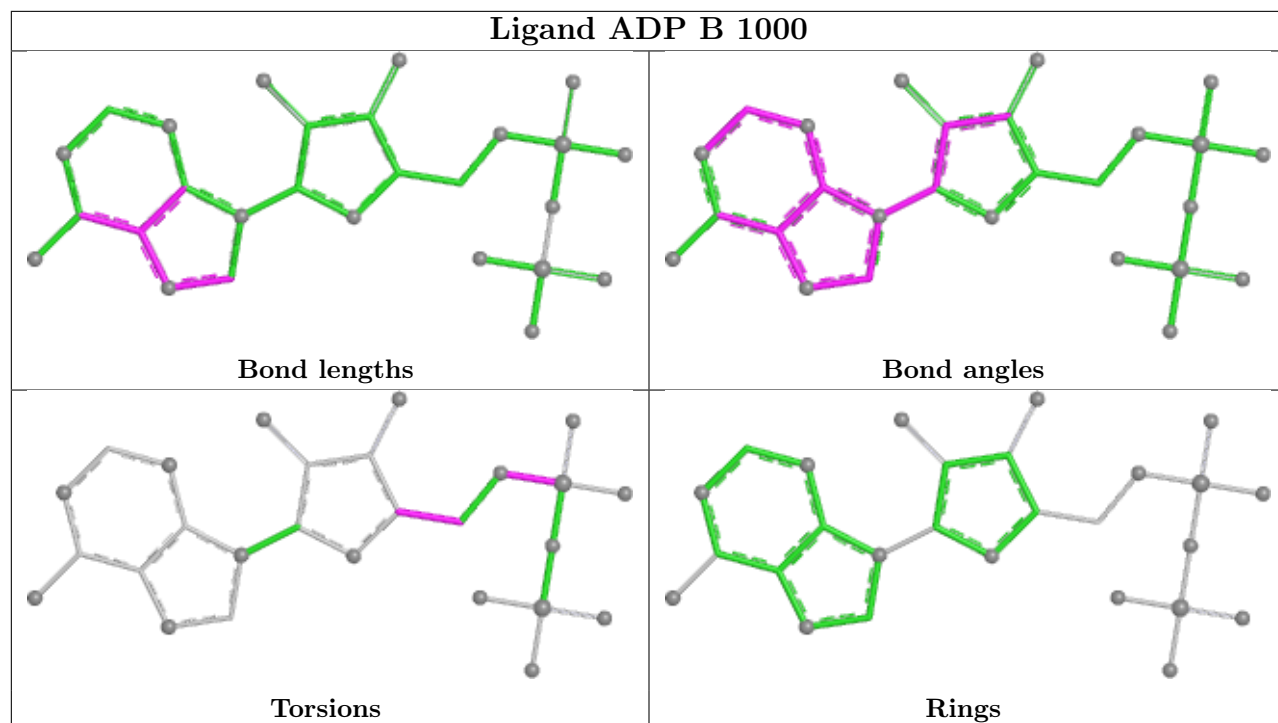
Mol	Chain	Res	Type	Atoms
3	B	1000	ADP	C5'-O5'-PA-O1A
3	C	1000	ADP	C5'-O5'-PA-O1A
3	D	1000	ADP	C5'-O5'-PA-O1A
3	A	1000	ADP	C3'-C4'-C5'-O5'
3	B	1000	ADP	C3'-C4'-C5'-O5'
3	C	1000	ADP	C3'-C4'-C5'-O5'
3	D	1000	ADP	C3'-C4'-C5'-O5'
3	E	1000	ADP	C3'-C4'-C5'-O5'
3	F	1000	ADP	C3'-C4'-C5'-O5'
3	C	1000	ADP	O4'-C4'-C5'-O5'
3	A	1000	ADP	O4'-C4'-C5'-O5'
3	B	1000	ADP	O4'-C4'-C5'-O5'
3	D	1000	ADP	O4'-C4'-C5'-O5'
3	E	1000	ADP	O4'-C4'-C5'-O5'
3	F	1000	ADP	O4'-C4'-C5'-O5'

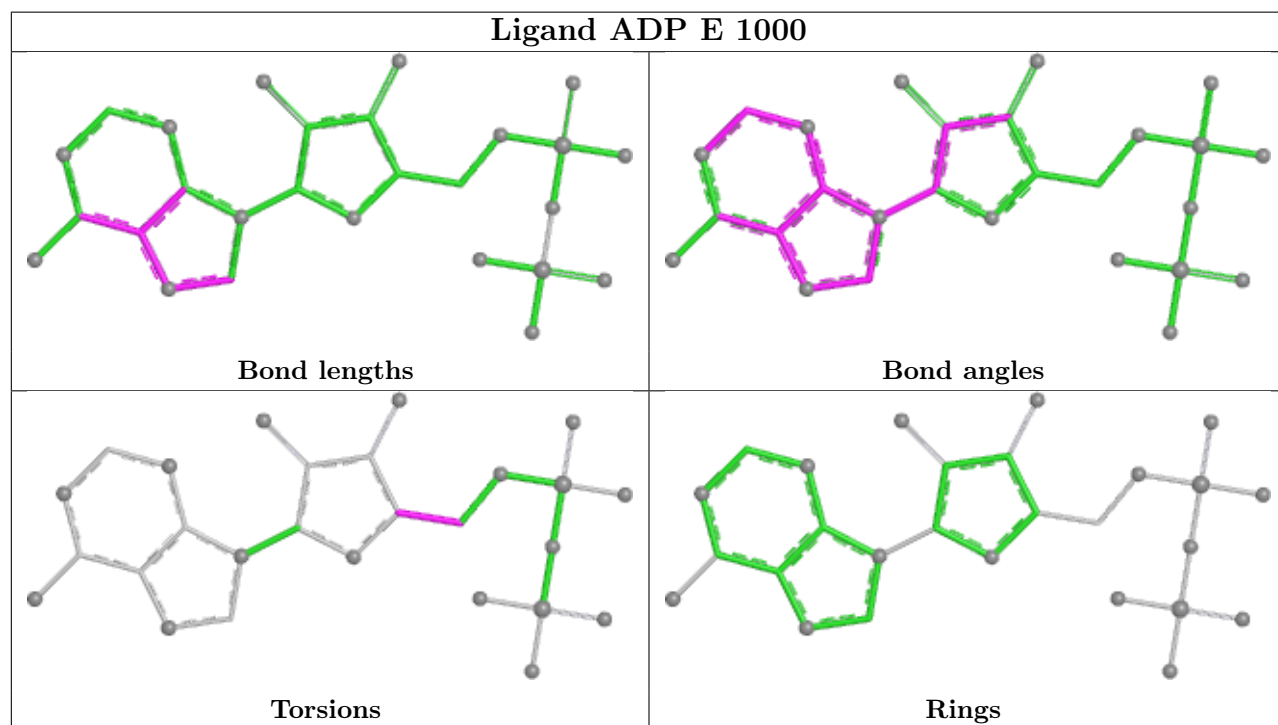
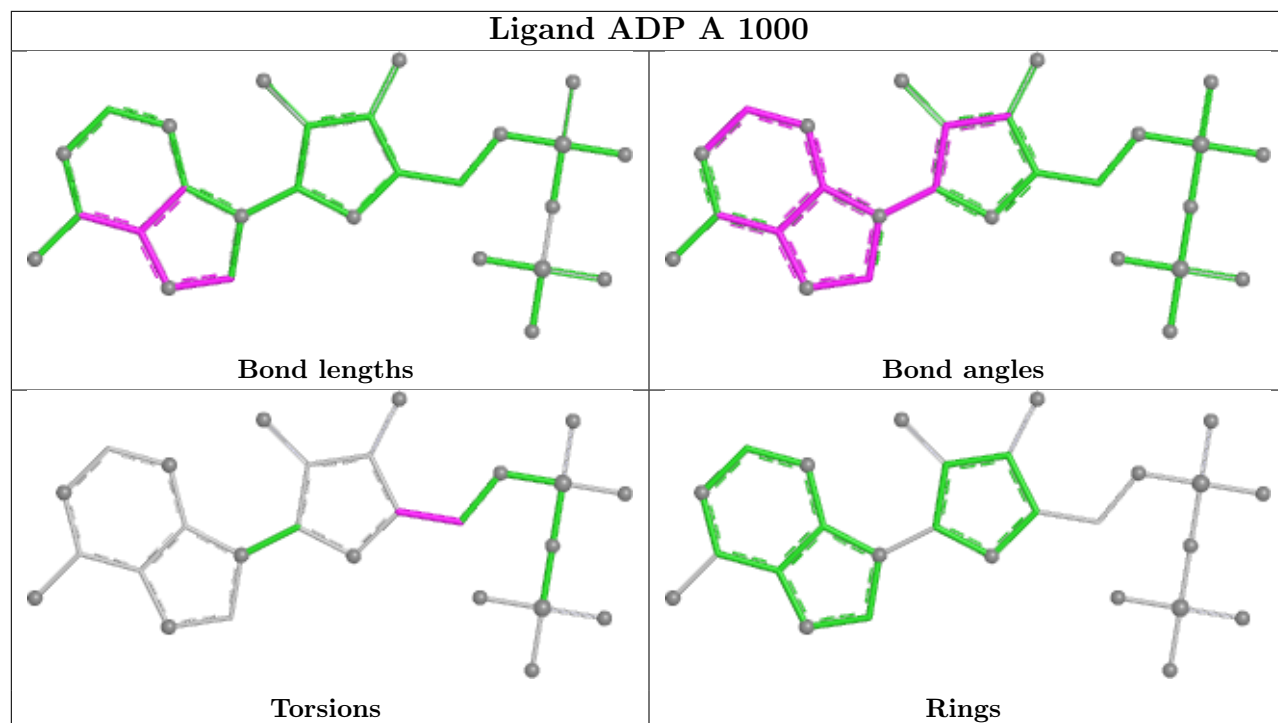
There are no ring outliers.

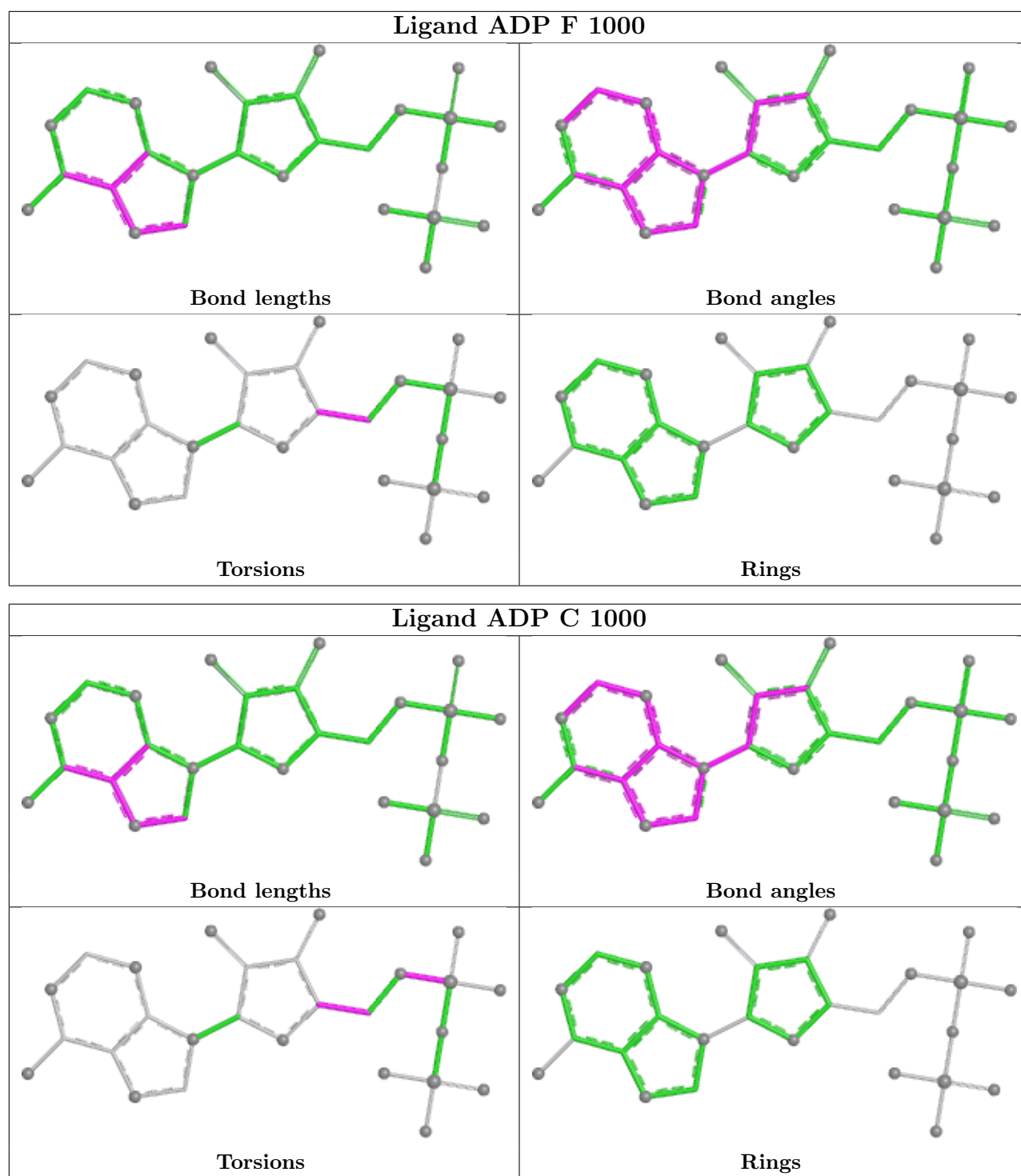
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	ADP	1	0
3	D	1000	ADP	1	0
3	A	1000	ADP	1	0
3	F	1000	ADP	1	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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	390/420 (92%)	0.03	2 (0%) 87 75	36, 68, 124, 149	0
1	B	394/420 (93%)	-0.08	0 100 100	24, 49, 127, 164	0
1	C	395/420 (94%)	-0.16	1 (0%) 90 81	22, 51, 113, 146	0
1	D	390/420 (92%)	0.14	4 (1%) 79 62	30, 73, 119, 163	0
1	E	343/420 (81%)	0.60	14 (4%) 41 24	67, 111, 154, 192	0
1	F	377/420 (89%)	0.44	6 (1%) 70 50	65, 98, 147, 177	0
2	G	7/12 (58%)	-0.21	0 100 100	47, 52, 88, 122	0
All	All	2296/2532 (90%)	0.15	27 (1%) 76 57	22, 76, 138, 192	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	321	ILE	3.4
1	E	342	GLU	3.3
1	F	294	LEU	3.2
1	E	289	VAL	2.9
1	E	116	VAL	2.8
1	E	127	ALA	2.7
1	D	142	ASN	2.6
1	E	98	SER	2.6
1	F	71	SER	2.5
1	D	322	ASP	2.5
1	E	143	SER	2.4
1	E	142	ASN	2.4
1	A	331	ILE	2.3
1	C	15	ILE	2.3
1	F	321	ILE	2.2
1	F	75	GLY	2.2
1	E	97	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	343	LEU	2.2
1	E	180	PRO	2.2
1	A	228	VAL	2.1
1	F	381	TRP	2.1
1	D	22	GLY	2.1
1	F	292	ASN	2.1
1	E	413	PHE	2.1
1	D	378	GLN	2.1
1	E	335	PHE	2.0
1	E	320	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	BEF	E	1002	4/4	0.81	0.17	115,117,117,118	0
3	ADP	E	1000	27/27	0.82	0.12	112,126,134,137	0
5	BEF	D	1002	4/4	0.90	0.09	78,81,81,83	0
3	ADP	F	1000	27/27	0.90	0.10	79,82,86,87	0
3	ADP	C	1000	27/27	0.91	0.11	45,56,63,64	0
5	BEF	C	1002	4/4	0.91	0.15	43,44,45,46	0
3	ADP	D	1000	27/27	0.92	0.09	60,77,86,88	0
3	ADP	B	1000	27/27	0.93	0.10	35,41,45,46	0
3	ADP	A	1000	27/27	0.94	0.08	39,43,49,49	0
5	BEF	B	1002	4/4	0.95	0.08	32,33,33,33	0
4	MG	E	1001	1/1	0.95	0.05	119,119,119,119	0
5	BEF	A	1002	4/4	0.96	0.07	45,45,45,46	0
5	BEF	F	1002	4/4	0.96	0.06	64,64,64,65	0

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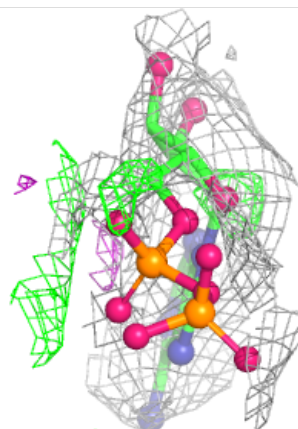
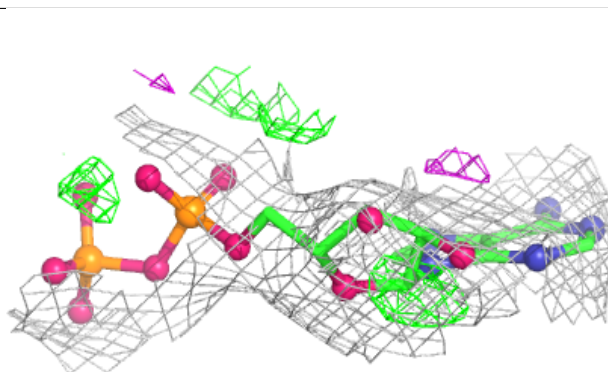
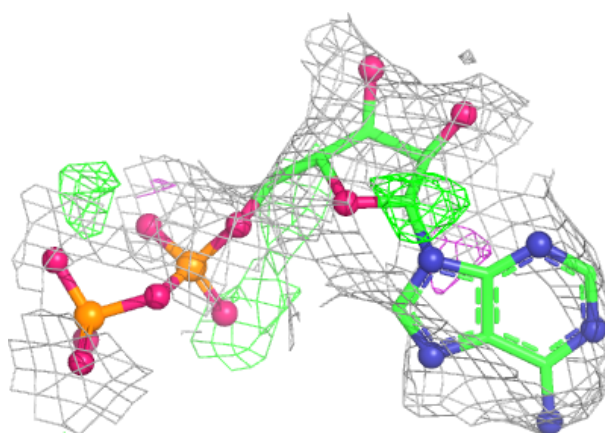
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	D	1001	1/1	0.98	0.07	97,97,97,97	0
4	MG	A	1001	1/1	0.99	0.04	36,36,36,36	0
4	MG	F	1001	1/1	0.99	0.03	64,64,64,64	0
4	MG	C	1001	1/1	1.00	0.05	37,37,37,37	0
4	MG	B	1001	1/1	1.00	0.03	26,26,26,26	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.

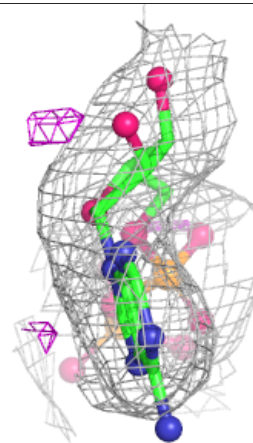
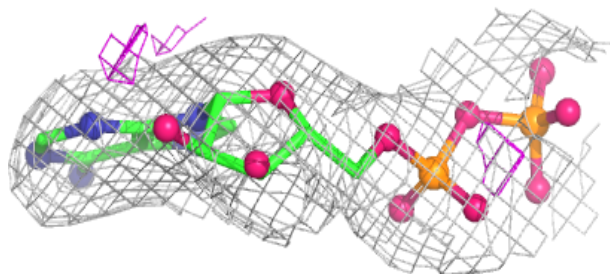
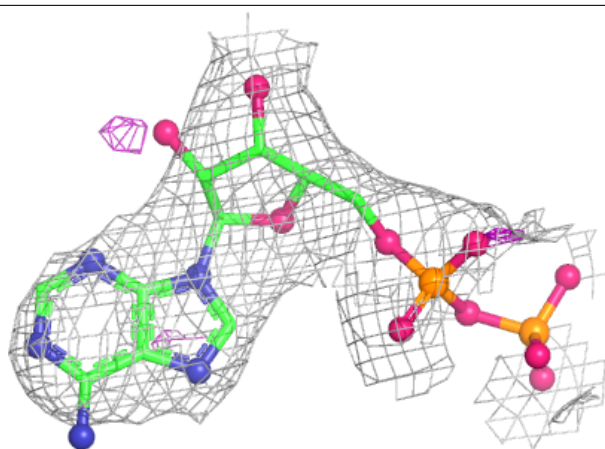
Electron density around ADP E 1000:

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



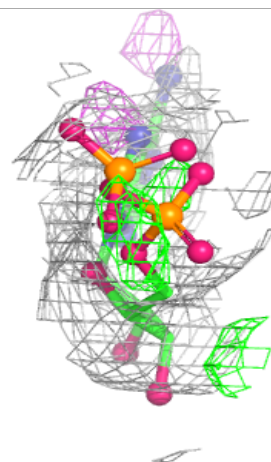
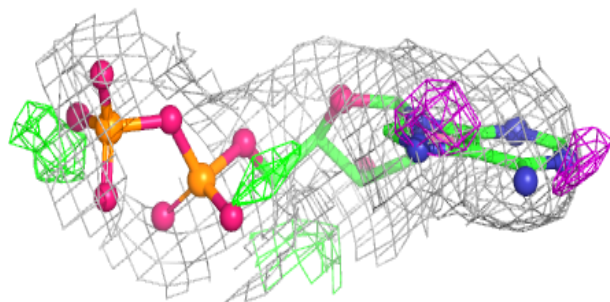
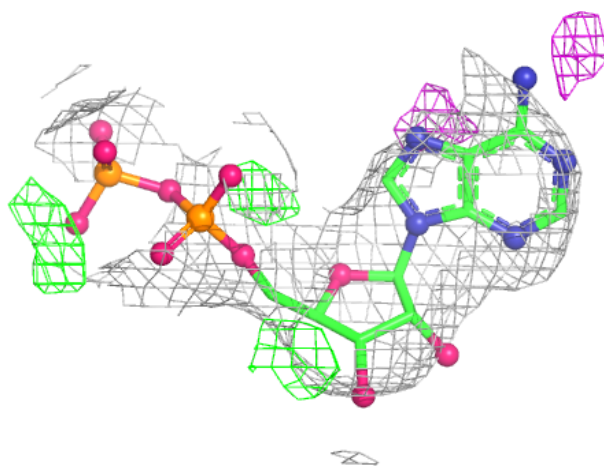
Electron density around ADP F 1000:

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



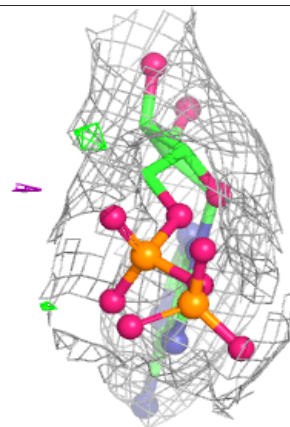
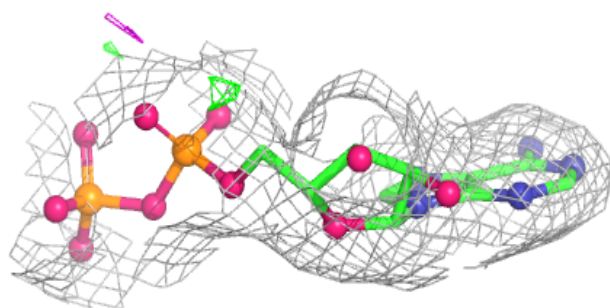
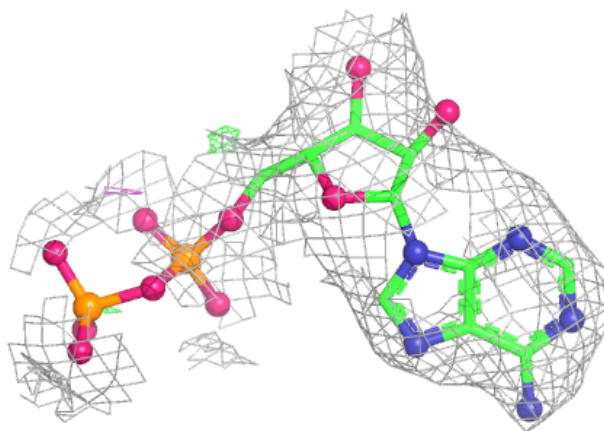
Electron density around ADP C 1000:

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



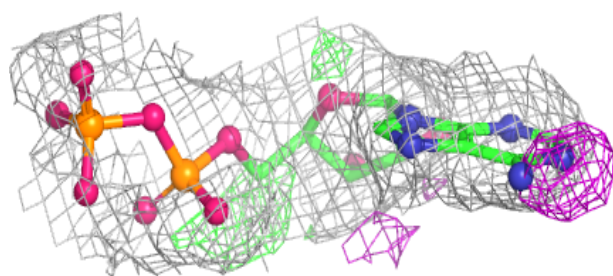
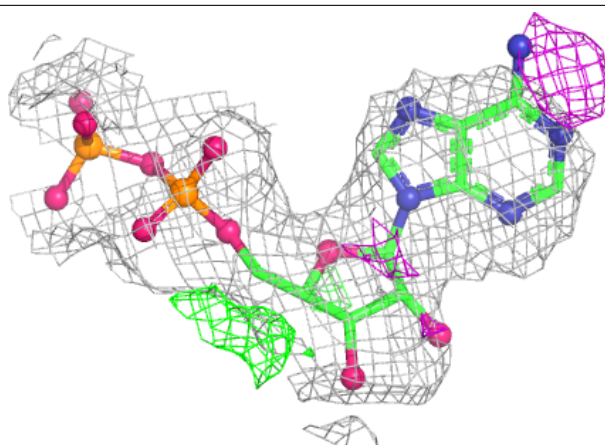
Electron density around ADP D 1000:

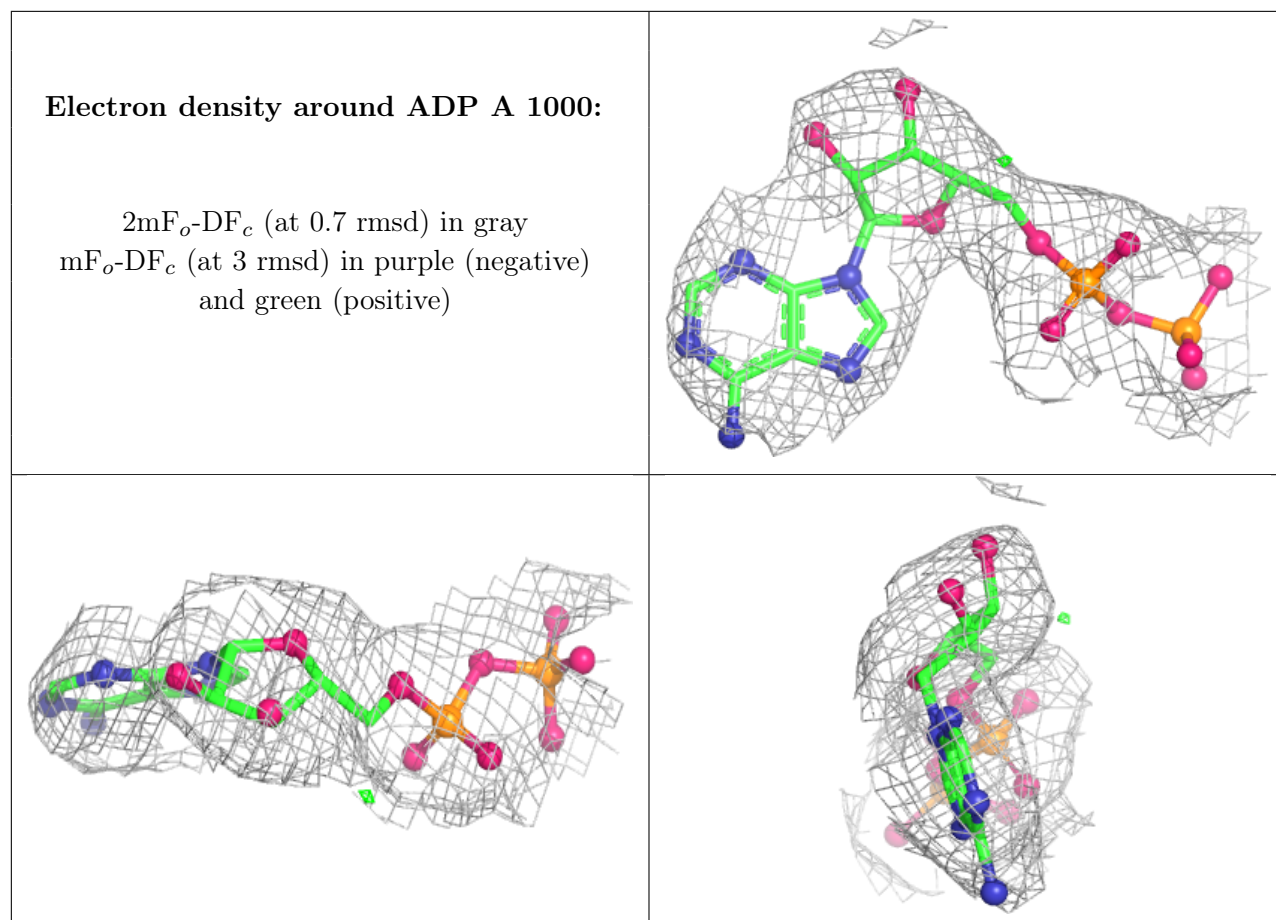
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP B 1000:

$2mF_o - DF_c$ (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.