



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:57 pm BST

PDB ID : 4IZ5
Title : Structure of the complex between ERK2 phosphomimetic mutant and PEA-15
Authors : Mace, P.D.; Robinson, H.; Riedl, S.J.
Deposited on : 2013-01-29
Resolution : 3.19 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

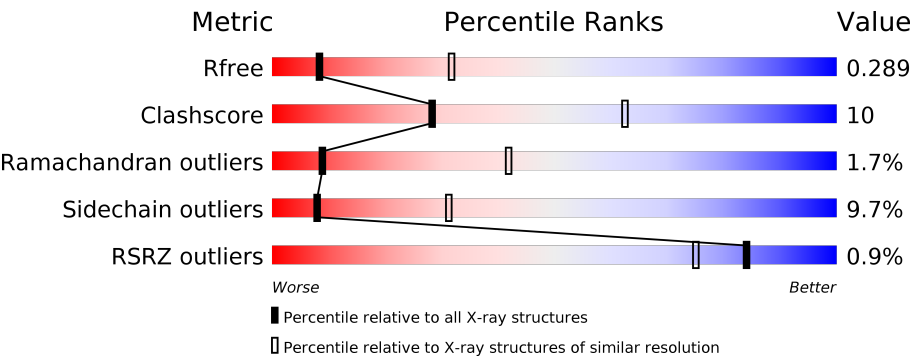
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	356	
1	B	356	
1	C	356	
1	D	356	
2	E	133	
2	F	133	

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Mol	Chain	Length	Quality of chain
2	G	133	
2	H	133	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	902	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14249 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 Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2836	1821	484	516	15			
1	B	347	Total	C	N	O	S	0	0	0
			2828	1816	483	514	15			
1	C	347	Total	C	N	O	S	0	0	0
			2836	1821	484	516	15			
1	D	347	Total	C	N	O	S	0	0	0
			2832	1819	484	514	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	EXPRESSION TAG	UNP P28482
A	6	PRO	-	EXPRESSION TAG	UNP P28482
A	7	GLY	-	EXPRESSION TAG	UNP P28482
A	185	GLU	THR	ENGINEERED MUTATION	UNP P28482
B	5	GLY	-	EXPRESSION TAG	UNP P28482
B	6	PRO	-	EXPRESSION TAG	UNP P28482
B	7	GLY	-	EXPRESSION TAG	UNP P28482
B	185	GLU	THR	ENGINEERED MUTATION	UNP P28482
C	5	GLY	-	EXPRESSION TAG	UNP P28482
C	6	PRO	-	EXPRESSION TAG	UNP P28482
C	7	GLY	-	EXPRESSION TAG	UNP P28482
C	185	GLU	THR	ENGINEERED MUTATION	UNP P28482
D	5	GLY	-	EXPRESSION TAG	UNP P28482
D	6	PRO	-	EXPRESSION TAG	UNP P28482
D	7	GLY	-	EXPRESSION TAG	UNP P28482
D	185	GLU	THR	ENGINEERED MUTATION	UNP P28482

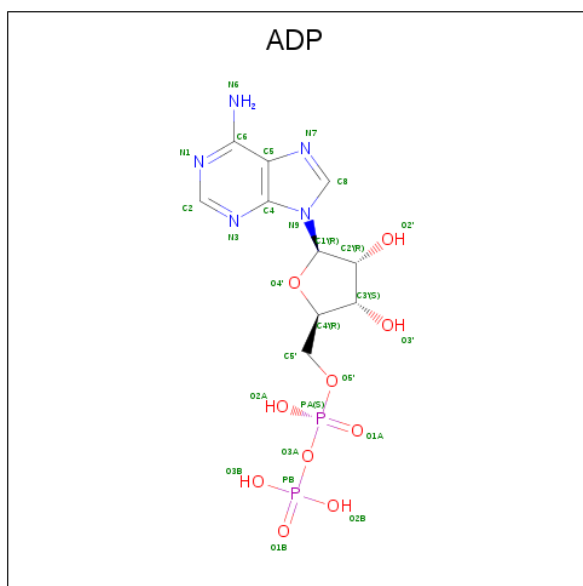
- Molecule 2 is a protein called Astrocytic phosphoprotein PEA-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	86	Total	C	N	O	S	0	0	0
			693	439	111	140	3			
2	F	86	Total	C	N	O	S	0	0	0
			693	439	111	140	3			
2	G	86	Total	C	N	O	S	0	0	0
			693	439	111	140	3			
2	H	80	Total	C	N	O	S	0	0	0
			650	409	104	134	3			

There are 12 discrepancies between the modelled and reference sequences:

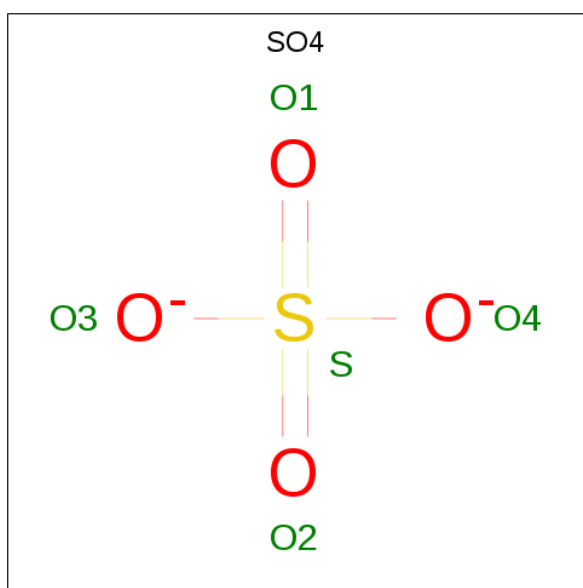
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP Q15121
E	-1	SER	-	EXPRESSION TAG	UNP Q15121
E	0	HIS	-	EXPRESSION TAG	UNP Q15121
F	-2	GLY	-	EXPRESSION TAG	UNP Q15121
F	-1	SER	-	EXPRESSION TAG	UNP Q15121
F	0	HIS	-	EXPRESSION TAG	UNP Q15121
G	-2	GLY	-	EXPRESSION TAG	UNP Q15121
G	-1	SER	-	EXPRESSION TAG	UNP Q15121
G	0	HIS	-	EXPRESSION TAG	UNP Q15121
H	-2	GLY	-	EXPRESSION TAG	UNP Q15121
H	-1	SER	-	EXPRESSION TAG	UNP Q15121
H	0	HIS	-	EXPRESSION TAG	UNP Q15121

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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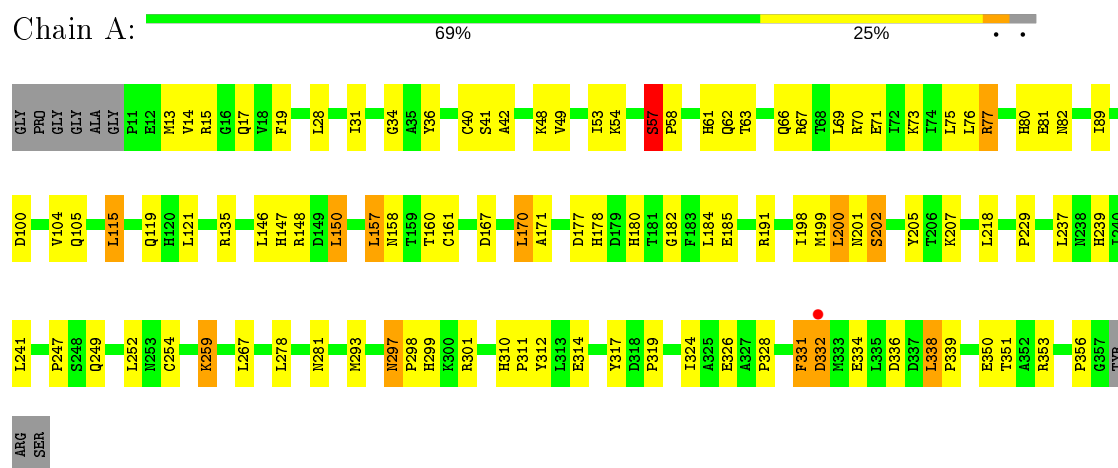
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

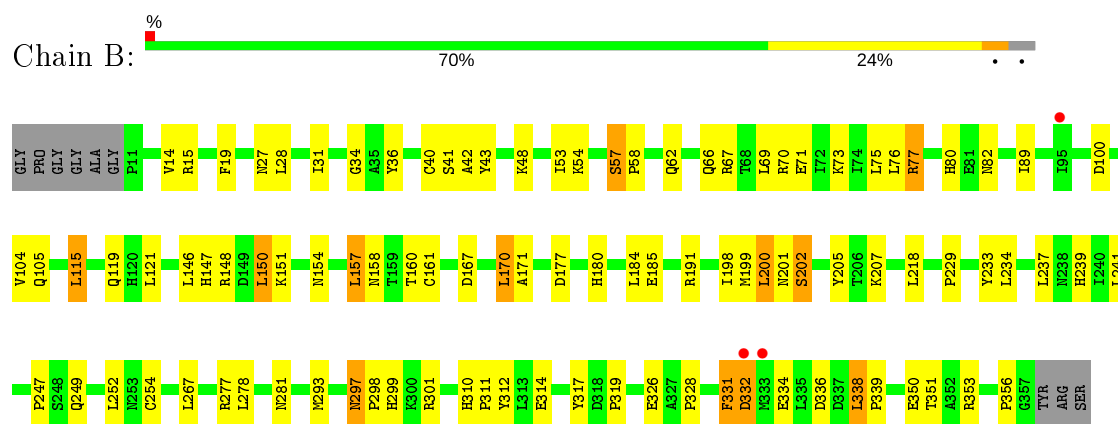
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

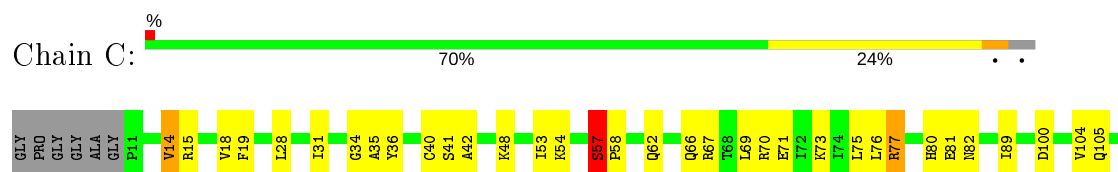
• Molecule 1: Mitogen-activated protein kinase 1

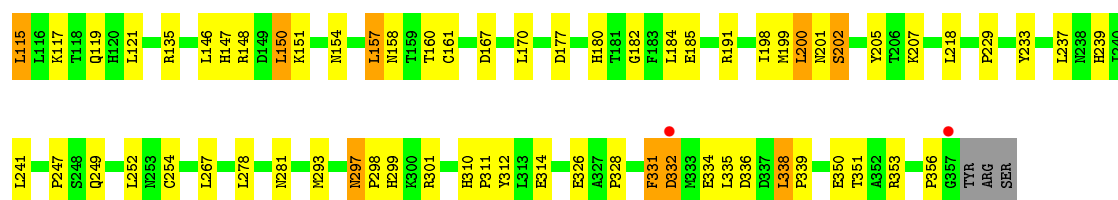


• Molecule 1: Mitogen-activated protein kinase 1

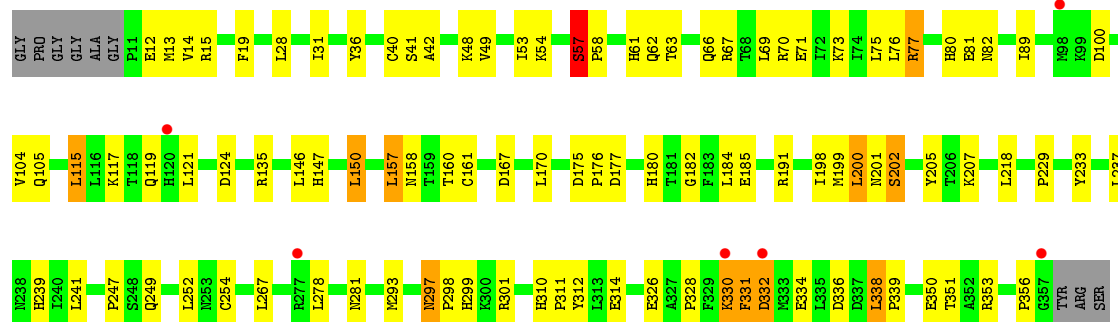


• Molecule 1: Mitogen-activated protein kinase 1

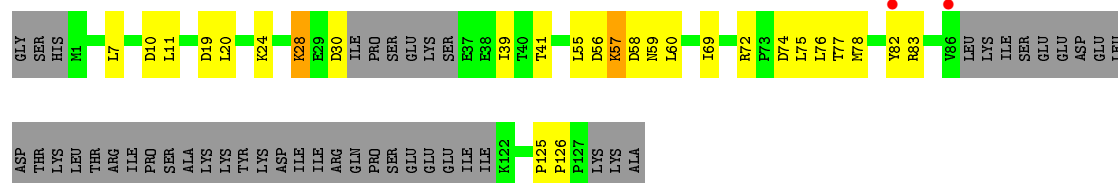
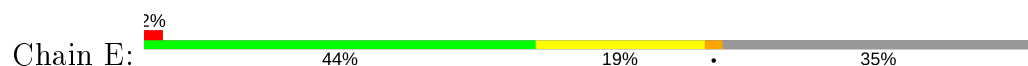




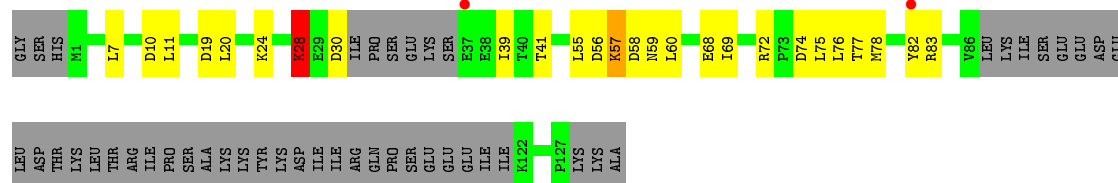
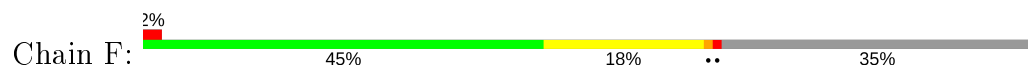
- Molecule 1: Mitogen-activated protein kinase 1



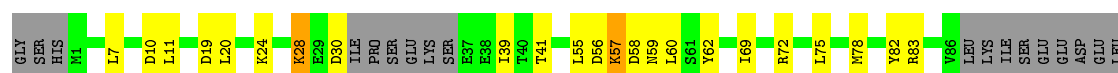
- Molecule 2: Astrocytic phosphoprotein PEA-15

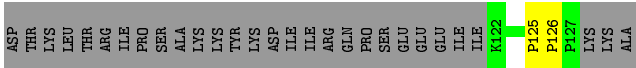


- Molecule 2: Astrocytic phosphoprotein PEA-15

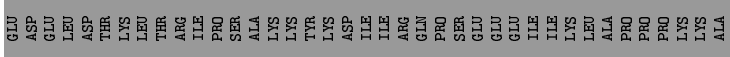
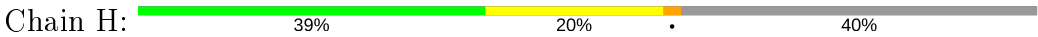


- Molecule 2: Astrocytic phosphoprotein PEA-15





● Molecule 2: Astrocytic phosphoprotein PEA-15



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.80Å 149.13Å 98.87Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	29.80 – 3.19 29.82 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.80-3.19) 96.8 (29.82-3.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0107	Depositor
R, R_{free}	0.243 , 0.292 0.243 , 0.289	Depositor DCC
R_{free} test set	1930 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 16.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.248 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14249	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: SO4, ADP

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	0.46	0/2905	0.57	2/3936 (0.1%)
1	B	0.47	0/2897	0.56	2/3927 (0.1%)
1	C	0.46	0/2905	0.56	2/3936 (0.1%)
1	D	0.46	0/2901	0.56	2/3931 (0.1%)
2	E	0.45	0/704	0.58	0/952
2	F	0.46	0/704	0.57	0/952
2	G	0.46	0/704	0.57	0/952
2	H	0.47	0/659	0.57	0/890
All	All	0.46	0/14379	0.56	8/19476 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	LEU	CA-CB-CG	6.58	130.43	115.30
1	D	157	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	157	LEU	CA-CB-CG	6.40	130.02	115.30
1	C	157	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	200	LEU	CA-CB-CG	5.94	128.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	LEU	CA-CB-CG	5.93	128.94	115.30
1	B	200	LEU	CA-CB-CG	5.70	128.42	115.30
1	D	200	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	SER	Peptide
1	C	57	SER	Peptide
1	D	57	SER	Peptide

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	2836	0	2835	58	0
1	B	2828	0	2820	56	0
1	C	2836	0	2835	53	0
1	D	2832	0	2831	56	0
2	E	693	0	676	17	0
2	F	693	0	676	17	0
2	G	693	0	676	18	0
2	H	650	0	627	19	0
3	A	27	0	12	3	0
3	B	27	0	12	2	0
3	C	27	0	12	3	0
3	D	27	0	12	2	0
4	A	20	0	0	2	0
4	B	20	0	0	1	0
4	C	20	0	0	2	0
4	D	20	0	0	1	0
All	All	14249	0	14024	278	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 10.

All (278) 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:D:57:SER:HB3	1:D:58:PRO:HD3	1.39	1.03
1:C:57:SER:HB3	1:C:58:PRO:HD3	1.38	1.03
1:B:57:SER:HB3	1:B:58:PRO:HD3	1.38	1.00
1:A:57:SER:HB3	1:A:58:PRO:HD3	1.40	0.99
1:C:80:HIS:HD2	1:C:82:ASN:H	1.28	0.81
1:B:80:HIS:HD2	1:B:82:ASN:H	1.30	0.80
1:A:80:HIS:HD2	1:A:82:ASN:H	1.29	0.80
1:C:57:SER:HB3	1:C:58:PRO:CD	2.13	0.78
1:B:57:SER:HB3	1:B:58:PRO:CD	2.14	0.78
1:A:57:SER:HB3	1:A:58:PRO:CD	2.16	0.75
1:D:80:HIS:HD2	1:D:82:ASN:H	1.31	0.75
1:D:57:SER:HB3	1:D:58:PRO:CD	2.16	0.75
1:A:34:GLY:CA	3:A:900:ADP:H5'1	2.17	0.74
2:G:57:LYS:H	2:G:57:LYS:HD2	1.54	0.73
1:C:80:HIS:CD2	1:C:82:ASN:H	2.08	0.71
2:E:57:LYS:H	2:E:57:LYS:HD2	1.55	0.71
1:D:338:LEU:HB2	1:D:339:PRO:HD2	1.73	0.71
1:A:338:LEU:HB2	1:A:339:PRO:HD2	1.73	0.70
1:B:80:HIS:CD2	1:B:82:ASN:H	2.09	0.70
1:B:233:TYR:HD2	2:H:76:LEU:HD23	1.57	0.70
2:H:57:LYS:H	2:H:57:LYS:HD2	1.56	0.70
1:D:73:LYS:HG3	1:D:350:GLU:OE2	1.92	0.70
1:A:17:GLN:HE22	1:B:58:PRO:HD2	1.56	0.69
1:D:80:HIS:CD2	1:D:82:ASN:H	2.10	0.69
2:E:7:LEU:HD22	2:E:82:TYR:HB2	1.75	0.69
1:A:80:HIS:CD2	1:A:82:ASN:H	2.08	0.69
1:C:338:LEU:HB2	1:C:339:PRO:HD2	1.75	0.69
1:D:14:VAL:HG11	1:D:40:CYS:SG	2.32	0.69
1:D:124:ASP:HB3	2:E:126:PRO:HG2	1.75	0.69
1:C:57:SER:CB	1:C:58:PRO:HD3	2.21	0.69
1:B:338:LEU:HB2	1:B:339:PRO:HD2	1.74	0.68
2:E:60:LEU:HD13	2:E:83:ARG:HD3	1.75	0.68
1:A:66:GLN:O	1:A:70:ARG:HG3	1.93	0.68
1:B:57:SER:CB	1:B:58:PRO:HD3	2.21	0.68
2:F:57:LYS:H	2:F:57:LYS:HD2	1.59	0.68
1:D:328:PRO:HG3	2:H:9:GLN:HE21	1.59	0.67
1:B:66:GLN:O	1:B:70:ARG:HG3	1.94	0.67
2:F:7:LEU:HD22	2:F:82:TYR:HB2	1.75	0.67
2:H:7:LEU:HD22	2:H:82:TYR:HB2	1.76	0.67
2:G:7:LEU:HD22	2:G:82:TYR:HB2	1.76	0.66
2:H:60:LEU:HD13	2:H:83:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:HD2	1:A:312:TYR:H	1.45	0.65
2:G:60:LEU:HD13	2:G:83:ARG:HD3	1.78	0.65
1:C:66:GLN:O	1:C:70:ARG:HG3	1.96	0.65
2:F:60:LEU:HD13	2:F:83:ARG:HD3	1.78	0.65
1:A:34:GLY:HA2	3:A:900:ADP:H5'1	1.79	0.64
2:E:10:ASP:HB3	2:E:78:MET:HE3	1.81	0.63
1:B:66:GLN:HG2	1:B:70:ARG:HH11	1.64	0.63
1:C:73:LYS:HG3	1:C:350:GLU:OE2	1.98	0.63
1:D:66:GLN:O	1:D:70:ARG:HG3	1.99	0.63
1:C:310:HIS:HD2	1:C:312:TYR:H	1.46	0.62
2:H:10:ASP:HB3	2:H:78:MET:HE3	1.80	0.62
1:B:310:HIS:HD2	1:B:312:TYR:H	1.47	0.62
1:A:73:LYS:HG3	1:A:350:GLU:OE2	2.00	0.61
1:B:73:LYS:HG3	1:B:350:GLU:OE2	1.99	0.61
1:D:36:TYR:OH	1:D:71:GLU:HG3	2.01	0.61
1:A:14:VAL:HG11	1:A:40:CYS:SG	2.40	0.61
1:D:330:LYS:HG3	2:H:2:ALA:O	2.00	0.61
1:A:57:SER:CB	1:A:58:PRO:HD3	2.22	0.60
1:D:297:ASN:HD22	1:D:299:HIS:H	1.49	0.60
1:A:297:ASN:HD22	1:A:299:HIS:H	1.50	0.59
1:B:36:TYR:OH	1:B:71:GLU:HG3	2.03	0.59
1:C:66:GLN:HG2	1:C:70:ARG:HH11	1.68	0.59
1:D:310:HIS:HD2	1:D:312:TYR:H	1.49	0.59
1:D:57:SER:CB	1:D:58:PRO:HD3	2.23	0.59
1:A:36:TYR:OH	1:A:71:GLU:HG3	2.03	0.59
1:C:297:ASN:HD22	1:C:299:HIS:H	1.50	0.59
1:D:76:LEU:HG	1:D:353:ARG:HH21	1.67	0.58
1:A:76:LEU:HG	1:A:353:ARG:HH21	1.68	0.58
1:D:66:GLN:HG2	1:D:70:ARG:HH11	1.68	0.58
2:G:10:ASP:HB3	2:G:78:MET:HE3	1.84	0.58
1:B:233:TYR:HD2	2:H:76:LEU:CD2	2.17	0.58
1:A:34:GLY:HA3	3:A:900:ADP:H5'1	1.86	0.57
1:C:147:HIS:ND1	1:C:150:LEU:HD13	2.19	0.57
1:A:66:GLN:HG2	1:A:70:ARG:HH11	1.68	0.57
1:C:14:VAL:HG11	1:C:40:CYS:SG	2.45	0.57
1:D:53:ILE:HG12	1:D:104:VAL:HG22	1.86	0.57
1:C:338:LEU:HB2	1:C:339:PRO:CD	2.35	0.57
1:D:338:LEU:HB2	1:D:339:PRO:CD	2.34	0.57
3:D:900:ADP:O1B	3:D:900:ADP:H5'2	2.05	0.57
1:C:36:TYR:OH	1:C:71:GLU:HG3	2.05	0.57
1:A:338:LEU:HB2	1:A:339:PRO:CD	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASN:HD22	1:B:299:HIS:H	1.52	0.56
1:B:338:LEU:HB2	1:B:339:PRO:CD	2.34	0.56
1:B:14:VAL:HG11	1:B:40:CYS:SG	2.46	0.56
1:A:310:HIS:CD2	1:A:312:TYR:H	2.23	0.56
1:B:254:CYS:SG	1:B:298:PRO:HD2	2.47	0.55
1:C:76:LEU:HG	1:C:353:ARG:HH21	1.71	0.54
1:C:70:ARG:NH2	4:C:901:SO4:O3	2.41	0.54
1:B:76:LEU:HG	1:B:353:ARG:HH21	1.71	0.53
2:F:10:ASP:HB3	2:F:78:MET:HE3	1.89	0.53
1:A:147:HIS:ND1	1:A:150:LEU:HD13	2.23	0.53
1:B:71:GLU:O	1:B:75:LEU:HB2	2.09	0.53
1:C:57:SER:CB	1:C:58:PRO:CD	2.85	0.53
1:C:71:GLU:O	1:C:75:LEU:HB2	2.08	0.53
1:B:36:TYR:CZ	1:B:71:GLU:HG3	2.45	0.52
1:D:147:HIS:ND1	1:D:150:LEU:HD13	2.25	0.52
1:A:57:SER:CB	1:A:58:PRO:CD	2.86	0.52
1:D:36:TYR:CZ	1:D:71:GLU:HG3	2.45	0.52
1:B:53:ILE:HG12	1:B:104:VAL:HG22	1.91	0.52
1:C:53:ILE:HG12	1:C:104:VAL:HG22	1.92	0.52
1:D:182:GLY:HA3	2:E:69:ILE:HD13	1.90	0.51
1:B:148:ARG:NH2	4:B:902:SO4:O3	2.44	0.51
1:C:148:ARG:NH2	4:C:902:SO4:O3	2.43	0.51
1:B:147:HIS:ND1	1:B:150:LEU:HD13	2.25	0.51
1:C:310:HIS:CD2	1:C:312:TYR:H	2.25	0.51
1:B:89:ILE:HD13	1:B:351:THR:HG22	1.92	0.51
1:C:36:TYR:CZ	1:C:71:GLU:HG3	2.46	0.51
2:E:56:ASP:HB2	2:E:59:ASN:CB	2.40	0.51
2:F:56:ASP:HB2	2:F:59:ASN:CB	2.41	0.51
1:A:71:GLU:O	1:A:75:LEU:HB2	2.11	0.51
1:A:13:MET:HB2	1:A:17:GLN:O	2.11	0.51
1:A:53:ILE:HG12	1:A:104:VAL:HG22	1.93	0.51
1:A:36:TYR:CZ	1:A:71:GLU:HG3	2.46	0.51
1:C:254:CYS:SG	1:C:298:PRO:HD2	2.50	0.51
1:A:259:LYS:NZ	2:G:19:ASP:OD2	2.44	0.51
1:D:310:HIS:CD2	1:D:312:TYR:H	2.28	0.51
1:A:66:GLN:HE21	1:A:70:ARG:NH1	2.09	0.50
1:B:234:LEU:HD12	2:H:80:VAL:HG21	1.93	0.50
1:B:57:SER:CB	1:B:58:PRO:CD	2.85	0.50
1:C:35:ALA:N	3:C:900:ADP:O1A	2.42	0.50
2:H:56:ASP:HB2	2:H:59:ASN:CB	2.42	0.50
1:C:198:ILE:HA	1:C:205:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLY:HA3	2:F:69:ILE:HD13	1.94	0.50
1:D:66:GLN:HE21	1:D:70:ARG:NH1	2.09	0.50
1:A:198:ILE:HA	1:A:205:TYR:CE1	2.47	0.49
1:B:310:HIS:CD2	1:B:312:TYR:H	2.26	0.49
1:B:28:LEU:HD13	1:B:42:ALA:HB2	1.94	0.49
1:A:241:LEU:HD22	1:A:247:PRO:HD3	1.94	0.49
1:D:89:ILE:HD13	1:D:351:THR:HG22	1.93	0.49
1:D:146:LEU:CD2	1:D:207:LYS:HA	2.41	0.49
2:G:20:LEU:HD13	2:G:24:LYS:HE3	1.93	0.49
1:A:146:LEU:CD2	1:A:207:LYS:HA	2.42	0.49
2:G:56:ASP:HB2	2:G:59:ASN:CB	2.42	0.49
1:A:254:CYS:SG	1:A:298:PRO:HD2	2.53	0.49
1:D:254:CYS:SG	1:D:298:PRO:HD2	2.52	0.49
1:D:71:GLU:O	1:D:75:LEU:HB2	2.13	0.49
2:F:20:LEU:HD13	2:F:24:LYS:HE3	1.95	0.49
1:A:148:ARG:NH2	4:A:902:SO4:O2	2.37	0.48
1:C:146:LEU:CD2	1:C:207:LYS:HA	2.43	0.48
3:B:900:ADP:O1B	3:B:900:ADP:H5'2	2.13	0.48
2:E:11:LEU:HD23	2:E:78:MET:HE2	1.95	0.48
1:A:326:GLU:O	1:A:328:PRO:HD3	2.14	0.48
1:B:54:LYS:NZ	1:B:105:GLN:OE1	2.46	0.48
1:C:66:GLN:HE21	1:C:70:ARG:NH1	2.12	0.48
2:H:57:LYS:H	2:H:57:LYS:CD	2.26	0.48
1:C:89:ILE:HD13	1:C:351:THR:HG22	1.94	0.48
1:A:28:LEU:HD13	1:A:42:ALA:HB2	1.96	0.48
1:C:28:LEU:HD13	1:C:42:ALA:HB2	1.95	0.48
2:E:56:ASP:HB2	2:E:59:ASN:HB3	1.95	0.48
2:H:20:LEU:HD13	2:H:24:LYS:HE3	1.94	0.48
1:A:77:ARG:CZ	1:A:331:PHE:CZ	2.97	0.48
1:A:89:ILE:HD13	1:A:351:THR:HG22	1.96	0.48
1:D:201:ASN:O	1:D:202:SER:CB	2.62	0.48
1:B:27:ASN:ND2	2:G:62:TYR:HB2	2.28	0.48
1:D:293:MET:O	1:D:301:ARG:HD2	2.14	0.47
2:F:56:ASP:HB2	2:F:59:ASN:HB3	1.96	0.47
2:H:56:ASP:HB2	2:H:59:ASN:HB3	1.96	0.47
1:D:28:LEU:HD13	1:D:42:ALA:HB2	1.96	0.47
1:D:330:LYS:HE2	2:H:5:GLY:HA3	1.97	0.47
2:F:11:LEU:HD23	2:F:78:MET:HE2	1.95	0.47
1:B:198:ILE:HA	1:B:205:TYR:CE1	2.49	0.47
1:C:201:ASN:O	1:C:202:SER:CB	2.62	0.47
1:D:198:ILE:HA	1:D:205:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLN:HE21	1:B:70:ARG:NH1	2.13	0.47
2:G:11:LEU:HD23	2:G:78:MET:HE2	1.96	0.47
1:A:201:ASN:O	1:A:202:SER:CB	2.62	0.47
1:C:241:LEU:HD22	1:C:247:PRO:HD3	1.97	0.47
1:B:146:LEU:CD2	1:B:207:LYS:HA	2.44	0.47
1:A:180:HIS:HE1	1:A:185:GLU:OE1	1.98	0.46
1:C:332:ASP:C	1:C:334:GLU:N	2.69	0.46
2:E:20:LEU:HD13	2:E:24:LYS:HE3	1.97	0.46
2:E:19:ASP:HB3	2:E:72:ARG:HH12	1.80	0.46
2:G:57:LYS:CD	2:G:57:LYS:H	2.24	0.46
1:D:201:ASN:O	1:D:202:SER:HB2	2.14	0.46
1:A:54:LYS:NZ	1:A:105:GLN:OE1	2.43	0.46
1:B:180:HIS:HE1	1:B:185:GLU:OE1	1.97	0.46
2:F:19:ASP:HB3	2:F:72:ARG:HH12	1.81	0.46
1:B:201:ASN:O	1:B:202:SER:CB	2.63	0.46
1:B:293:MET:O	1:B:301:ARG:HD2	2.15	0.46
1:D:311:PRO:O	1:D:314:GLU:HB2	2.15	0.46
2:H:19:ASP:HB3	2:H:72:ARG:HH12	1.80	0.46
1:D:180:HIS:HE1	1:D:185:GLU:OE1	1.99	0.46
1:A:115:LEU:HD11	1:A:121:LEU:HD21	1.98	0.46
1:B:148:ARG:HD3	1:B:170:LEU:O	2.16	0.46
1:B:31:ILE:HD11	1:B:41:SER:HB3	1.98	0.46
1:C:77:ARG:CZ	1:C:331:PHE:CZ	2.99	0.46
1:A:182:GLY:HA3	2:G:69:ILE:HD13	1.97	0.46
1:B:241:LEU:HD22	1:B:247:PRO:HD3	1.98	0.46
1:B:77:ARG:CZ	1:B:331:PHE:CZ	2.99	0.46
1:C:180:HIS:HE1	1:C:185:GLU:OE1	1.99	0.46
1:B:311:PRO:O	1:B:314:GLU:HB2	2.16	0.46
1:C:160:THR:O	1:C:161:CYS:HB2	2.16	0.46
1:D:115:LEU:HD11	1:D:121:LEU:HD21	1.98	0.46
1:B:229:PRO:HD2	1:B:239:HIS:ND1	2.31	0.45
1:B:332:ASP:C	1:B:334:GLU:N	2.70	0.45
1:A:332:ASP:C	1:A:334:GLU:N	2.70	0.45
1:D:54:LYS:NZ	1:D:105:GLN:OE1	2.45	0.45
1:D:241:LEU:HD22	1:D:247:PRO:HD3	1.98	0.45
1:D:57:SER:CB	1:D:58:PRO:CD	2.87	0.45
2:G:19:ASP:HB3	2:G:72:ARG:HH12	1.81	0.45
1:A:178:HIS:HE1	4:A:902:SO4:O1	2.00	0.45
2:E:57:LYS:H	2:E:57:LYS:CD	2.25	0.45
1:A:31:ILE:HD11	1:A:41:SER:HB3	1.99	0.45
1:C:115:LEU:HD11	1:C:121:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD11	1:B:121:LEU:HD21	1.98	0.45
1:D:332:ASP:C	1:D:334:GLU:N	2.69	0.45
1:A:311:PRO:O	1:A:314:GLU:HB2	2.16	0.44
1:C:233:TYR:CD1	2:F:68:GLU:HG3	2.53	0.44
1:A:293:MET:O	1:A:301:ARG:HD2	2.17	0.44
1:C:201:ASN:O	1:C:202:SER:HB2	2.16	0.44
1:A:229:PRO:HD2	1:A:239:HIS:ND1	2.32	0.44
1:D:326:GLU:O	1:D:328:PRO:HD3	2.18	0.44
1:C:34:GLY:HA2	3:C:900:ADP:H5'1	1.99	0.44
2:E:7:LEU:HA	2:E:10:ASP:HB2	2.00	0.44
1:C:311:PRO:O	1:C:314:GLU:HB2	2.17	0.44
1:C:326:GLU:O	1:C:328:PRO:HD3	2.18	0.44
1:A:148:ARG:HD3	1:A:170:LEU:O	2.17	0.44
1:B:160:THR:O	1:B:161:CYS:HB2	2.17	0.44
1:D:77:ARG:CZ	1:D:331:PHE:CZ	3.00	0.44
1:B:43:TYR:CZ	2:G:59:ASN:HB2	2.53	0.44
1:B:326:GLU:O	1:B:328:PRO:HD3	2.17	0.44
2:G:56:ASP:HB2	2:G:59:ASN:HB3	2.00	0.44
2:G:7:LEU:HA	2:G:10:ASP:HB2	1.98	0.44
2:H:11:LEU:HD23	2:H:78:MET:HE2	2.00	0.44
1:D:31:ILE:HD11	1:D:41:SER:HB3	1.99	0.43
1:D:36:TYR:OH	1:D:71:GLU:CG	2.65	0.43
1:C:293:MET:O	1:C:301:ARG:HD2	2.18	0.43
1:C:117:LYS:HE3	1:D:117:LYS:HE3	2.00	0.43
1:A:201:ASN:O	1:A:202:SER:HB2	2.18	0.43
1:D:233:TYR:HD2	2:E:76:LEU:HD23	1.84	0.43
1:B:201:ASN:O	1:B:202:SER:HB2	2.17	0.43
1:B:36:TYR:OH	1:B:71:GLU:CG	2.66	0.43
1:A:81:GLU:HB2	1:A:135:ARG:HH12	1.83	0.42
1:B:34:GLY:CA	3:B:900:ADP:H5'1	2.49	0.42
1:C:229:PRO:HD2	1:C:239:HIS:ND1	2.33	0.42
1:D:175:ASP:HA	1:D:176:PRO:HD2	1.94	0.42
2:F:7:LEU:HA	2:F:10:ASP:HB2	2.01	0.42
1:B:89:ILE:HG21	1:B:351:THR:CG2	2.49	0.42
1:C:81:GLU:HB2	1:C:135:ARG:HH12	1.85	0.42
1:D:160:THR:O	1:D:161:CYS:HB2	2.19	0.42
1:C:77:ARG:NH1	1:C:331:PHE:HZ	2.18	0.42
2:E:56:ASP:HB3	2:E:58:ASP:H	1.85	0.42
2:H:7:LEU:HA	2:H:10:ASP:HB2	2.01	0.42
1:B:151:LYS:HE2	1:B:154:ASN:ND2	2.35	0.42
2:H:56:ASP:HB3	2:H:58:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLY:CA	3:C:900:ADP:H5'1	2.50	0.42
2:H:74:ASP:O	2:H:77:THR:HG22	2.20	0.41
1:B:77:ARG:NH1	1:B:331:PHE:HZ	2.18	0.41
1:C:31:ILE:HD11	1:C:41:SER:HB3	2.01	0.41
2:E:125:PRO:HA	2:E:126:PRO:HD3	1.84	0.41
2:E:74:ASP:O	2:E:77:THR:HG22	2.21	0.41
2:F:56:ASP:HB3	2:F:58:ASP:H	1.86	0.41
2:F:74:ASP:O	2:F:77:THR:HG22	2.20	0.41
2:G:7:LEU:HG	2:G:10:ASP:OD2	2.20	0.41
1:A:146:LEU:O	1:A:171:ALA:HA	2.20	0.41
1:A:36:TYR:OH	1:A:71:GLU:CG	2.67	0.41
1:A:61:HIS:CE1	1:A:63:THR:OG1	2.73	0.41
1:B:146:LEU:O	1:B:171:ALA:HA	2.21	0.41
1:D:70:ARG:NH2	4:D:901:SO4:O3	2.53	0.41
2:G:56:ASP:HB3	2:G:58:ASP:H	1.85	0.41
1:D:229:PRO:HD2	1:D:239:HIS:ND1	2.34	0.41
1:D:61:HIS:CE1	1:D:63:THR:OG1	2.74	0.41
1:C:54:LYS:NZ	1:C:105:GLN:OE1	2.46	0.41
1:D:81:GLU:HB2	1:D:135:ARG:HH12	1.86	0.41
1:A:160:THR:O	1:A:161:CYS:HB2	2.20	0.41
1:A:77:ARG:NH1	1:A:331:PHE:HZ	2.18	0.41
1:C:233:TYR:HD2	2:F:76:LEU:HD23	1.86	0.41
2:F:57:LYS:H	2:F:57:LYS:CD	2.28	0.41
1:B:317:TYR:CZ	1:B:319:PRO:HG3	2.56	0.40
1:A:317:TYR:CZ	1:A:319:PRO:HG3	2.55	0.40
1:D:77:ARG:NH1	1:D:331:PHE:HZ	2.19	0.40
2:F:28:LYS:HA	2:F:28:LYS:HD2	1.94	0.40
1:D:54:LYS:NZ	3:D:900:ADP:N7	2.69	0.40
2:G:125:PRO:HA	2:G:126:PRO:HD3	1.81	0.40
1:A:324:ILE:HG13	1:A:324:ILE:H	1.76	0.40
1:C:151:LYS:HE2	1:C:154:ASN:ND2	2.37	0.40
1:D:12:GLU:CD	1:D:28:LEU:HD23	2.42	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	345/356 (97%)	320 (93%)	20 (6%)	5 (1%)	11	46
1	B	345/356 (97%)	319 (92%)	21 (6%)	5 (1%)	11	46
1	C	345/356 (97%)	320 (93%)	19 (6%)	6 (2%)	9	42
1	D	345/356 (97%)	320 (93%)	20 (6%)	5 (1%)	11	46
2	E	80/133 (60%)	74 (92%)	4 (5%)	2 (2%)	5	32
2	F	80/133 (60%)	74 (92%)	4 (5%)	2 (2%)	5	32
2	G	80/133 (60%)	73 (91%)	5 (6%)	2 (2%)	5	32
2	H	76/133 (57%)	69 (91%)	5 (7%)	2 (3%)	5	31
All	All	1696/1956 (87%)	1569 (92%)	98 (6%)	29 (2%)	9	42

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	B	57	SER
1	C	57	SER
1	D	57	SER
2	E	39	ILE
2	F	39	ILE
2	G	39	ILE
2	H	39	ILE
2	E	28	LYS
2	F	28	LYS
2	G	28	LYS
2	H	28	LYS
1	A	336	ASP
1	B	336	ASP
1	C	336	ASP
1	D	336	ASP
1	A	167	ASP
1	C	167	ASP
1	A	332	ASP
1	B	167	ASP
1	B	332	ASP
1	C	332	ASP
1	D	167	ASP

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Mol	Chain	Res	Type
1	C	335	LEU
1	D	332	ASP
1	A	356	PRO
1	B	356	PRO
1	C	356	PRO
1	D	356	PRO

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	314/318 (99%)	282 (90%)	32 (10%)	7	29
1	B	312/318 (98%)	281 (90%)	31 (10%)	8	30
1	C	314/318 (99%)	282 (90%)	32 (10%)	7	29
1	D	313/318 (98%)	280 (90%)	33 (10%)	7	28
2	E	79/124 (64%)	73 (92%)	6 (8%)	13	45
2	F	79/124 (64%)	73 (92%)	6 (8%)	13	45
2	G	79/124 (64%)	73 (92%)	6 (8%)	13	45
2	H	74/124 (60%)	68 (92%)	6 (8%)	11	42
All	All	1564/1768 (88%)	1412 (90%)	152 (10%)	8	31

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	19	PHE
1	A	48	LYS
1	A	49	VAL
1	A	62	GLN
1	A	67	ARG
1	A	69	LEU
1	A	77	ARG
1	A	100	ASP

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	119	GLN
1	A	150	LEU
1	A	157	LEU
1	A	158	ASN
1	A	170	LEU
1	A	177	ASP
1	A	184	LEU
1	A	191	ARG
1	A	199	MET
1	A	200	LEU
1	A	202	SER
1	A	218	LEU
1	A	237	LEU
1	A	249	GLN
1	A	252	LEU
1	A	259	LYS
1	A	267	LEU
1	A	278	LEU
1	A	281	ASN
1	A	297	ASN
1	A	331	PHE
1	A	338	LEU
1	B	15	ARG
1	B	19	PHE
1	B	48	LYS
1	B	62	GLN
1	B	67	ARG
1	B	69	LEU
1	B	77	ARG
1	B	100	ASP
1	B	115	LEU
1	B	119	GLN
1	B	150	LEU
1	B	157	LEU
1	B	158	ASN
1	B	170	LEU
1	B	177	ASP
1	B	184	LEU
1	B	191	ARG
1	B	199	MET
1	B	200	LEU

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Mol	Chain	Res	Type
1	B	202	SER
1	B	218	LEU
1	B	237	LEU
1	B	249	GLN
1	B	252	LEU
1	B	267	LEU
1	B	277	ARG
1	B	278	LEU
1	B	281	ASN
1	B	297	ASN
1	B	331	PHE
1	B	338	LEU
1	C	14	VAL
1	C	15	ARG
1	C	18	VAL
1	C	19	PHE
1	C	48	LYS
1	C	62	GLN
1	C	67	ARG
1	C	69	LEU
1	C	77	ARG
1	C	100	ASP
1	C	115	LEU
1	C	119	GLN
1	C	150	LEU
1	C	157	LEU
1	C	158	ASN
1	C	170	LEU
1	C	177	ASP
1	C	184	LEU
1	C	191	ARG
1	C	199	MET
1	C	200	LEU
1	C	202	SER
1	C	218	LEU
1	C	237	LEU
1	C	249	GLN
1	C	252	LEU
1	C	267	LEU
1	C	278	LEU
1	C	281	ASN
1	C	297	ASN

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Mol	Chain	Res	Type
1	C	331	PHE
1	C	338	LEU
1	D	13	MET
1	D	15	ARG
1	D	19	PHE
1	D	48	LYS
1	D	49	VAL
1	D	62	GLN
1	D	67	ARG
1	D	69	LEU
1	D	77	ARG
1	D	100	ASP
1	D	115	LEU
1	D	119	GLN
1	D	150	LEU
1	D	157	LEU
1	D	158	ASN
1	D	170	LEU
1	D	177	ASP
1	D	184	LEU
1	D	191	ARG
1	D	199	MET
1	D	200	LEU
1	D	202	SER
1	D	218	LEU
1	D	237	LEU
1	D	249	GLN
1	D	252	LEU
1	D	267	LEU
1	D	278	LEU
1	D	281	ASN
1	D	297	ASN
1	D	330	LYS
1	D	331	PHE
1	D	338	LEU
2	E	28	LYS
2	E	30	ASP
2	E	41	THR
2	E	55	LEU
2	E	57	LYS
2	E	75	LEU
2	F	28	LYS

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Mol	Chain	Res	Type
2	F	30	ASP
2	F	41	THR
2	F	55	LEU
2	F	57	LYS
2	F	75	LEU
2	G	28	LYS
2	G	30	ASP
2	G	41	THR
2	G	55	LEU
2	G	57	LYS
2	G	75	LEU
2	H	28	LYS
2	H	30	ASP
2	H	41	THR
2	H	55	LEU
2	H	57	LYS
2	H	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	47	ASN
1	A	61	HIS
1	A	62	GLN
1	A	66	GLN
1	A	80	HIS
1	A	87	ASN
1	A	178	HIS
1	A	180	HIS
1	A	238	ASN
1	A	249	GLN
1	A	297	ASN
1	A	306	GLN
1	A	310	HIS
1	B	17	GLN
1	B	47	ASN
1	B	61	HIS
1	B	62	GLN
1	B	66	GLN
1	B	80	HIS
1	B	87	ASN

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Mol	Chain	Res	Type
1	B	178	HIS
1	B	180	HIS
1	B	238	ASN
1	B	249	GLN
1	B	297	ASN
1	B	306	GLN
1	B	310	HIS
1	C	47	ASN
1	C	61	HIS
1	C	62	GLN
1	C	66	GLN
1	C	80	HIS
1	C	87	ASN
1	C	180	HIS
1	C	238	ASN
1	C	249	GLN
1	C	297	ASN
1	C	306	GLN
1	C	310	HIS
1	D	47	ASN
1	D	61	HIS
1	D	62	GLN
1	D	66	GLN
1	D	80	HIS
1	D	87	ASN
1	D	180	HIS
1	D	238	ASN
1	D	249	GLN
1	D	297	ASN
1	D	306	GLN
1	D	310	HIS
2	H	9	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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
3	ADP	C	900	-	24,29,29	1.28	5 (20%)	29,45,45	1.74	3 (10%)
4	SO4	A	904	-	4,4,4	0.36	0	6,6,6	0.10	0
4	SO4	C	903	-	4,4,4	0.38	0	6,6,6	0.25	0
3	ADP	B	900	-	24,29,29	1.25	4 (16%)	29,45,45	1.65	5 (17%)
4	SO4	A	903	-	4,4,4	0.29	0	6,6,6	0.11	0
3	ADP	A	900	-	24,29,29	1.33	5 (20%)	29,45,45	1.79	5 (17%)
3	ADP	D	900	-	24,29,29	1.29	5 (20%)	29,45,45	1.66	3 (10%)
4	SO4	B	902	-	4,4,4	0.30	0	6,6,6	0.25	0
4	SO4	D	901	-	4,4,4	0.29	0	6,6,6	0.26	0
4	SO4	C	902	-	4,4,4	0.31	0	6,6,6	0.29	0
4	SO4	B	901	-	4,4,4	0.26	0	6,6,6	0.27	0
4	SO4	D	902	-	4,4,4	0.30	0	6,6,6	0.25	0
4	SO4	A	901	-	4,4,4	0.33	0	6,6,6	0.21	0
4	SO4	D	903	-	4,4,4	0.29	0	6,6,6	0.16	0
4	SO4	C	901	-	4,4,4	0.34	0	6,6,6	0.22	0
4	SO4	B	904	-	4,4,4	0.36	0	6,6,6	0.06	0
4	SO4	A	902	-	4,4,4	0.33	0	6,6,6	0.24	0
4	SO4	B	903	-	4,4,4	0.33	0	6,6,6	0.13	0
4	SO4	D	904	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	C	904	-	4,4,4	0.33	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	900	-	-	3/12/32/32	0/3/3/3
3	ADP	D	900	-	-	4/12/32/32	0/3/3/3
3	ADP	A	900	-	-	3/12/32/32	0/3/3/3
3	ADP	B	900	-	-	4/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	ADP	PB-O3B	2.95	1.66	1.54
3	C	900	ADP	PB-O3B	2.89	1.66	1.54
3	A	900	ADP	PB-O2B	2.84	1.65	1.54
3	D	900	ADP	PB-O3B	2.84	1.65	1.54
3	D	900	ADP	PB-O2B	2.82	1.65	1.54
3	B	900	ADP	PB-O2B	2.79	1.65	1.54
3	B	900	ADP	PB-O3B	2.79	1.65	1.54
3	C	900	ADP	PB-O2B	2.79	1.65	1.54
3	A	900	ADP	O4'-C1'	2.34	1.44	1.41
3	A	900	ADP	C2-N3	2.33	1.35	1.32
3	D	900	ADP	O4'-C1'	2.32	1.44	1.41
3	B	900	ADP	PA-O2A	2.24	1.65	1.55
3	A	900	ADP	PA-O2A	2.23	1.65	1.55
3	C	900	ADP	PA-O2A	2.19	1.65	1.55
3	C	900	ADP	O4'-C1'	2.16	1.44	1.41
3	D	900	ADP	C2-N3	2.15	1.35	1.32
3	D	900	ADP	PA-O2A	2.12	1.65	1.55
3	C	900	ADP	C2-N3	2.05	1.35	1.32
3	B	900	ADP	O4'-C1'	2.01	1.43	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	ADP	PA-O3A-PB	-6.55	110.34	132.83
3	C	900	ADP	PA-O3A-PB	-6.22	111.47	132.83
3	D	900	ADP	PA-O3A-PB	-5.64	113.48	132.83
3	B	900	ADP	PA-O3A-PB	-5.24	114.84	132.83
3	B	900	ADP	N3-C2-N1	-4.86	121.08	128.68
3	C	900	ADP	N3-C2-N1	-4.84	121.12	128.68
3	D	900	ADP	N3-C2-N1	-4.67	121.38	128.68
3	A	900	ADP	N3-C2-N1	-4.35	121.89	128.68
3	B	900	ADP	C4-C5-N7	-2.23	107.07	109.40
3	A	900	ADP	C4-C5-N7	-2.22	107.08	109.40
3	A	900	ADP	PA-O5'-C5'	-2.22	108.67	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	900	ADP	C4-C5-N7	-2.21	107.10	109.40
3	B	900	ADP	O3B-PB-O3A	2.21	112.03	104.64
3	A	900	ADP	O4'-C1'-C2'	-2.10	103.86	106.93
3	B	900	ADP	PA-O5'-C5'	-2.09	109.43	121.68
3	D	900	ADP	PA-O5'-C5'	-2.08	109.50	121.68

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	900	ADP	C5'-O5'-PA-O1A
3	C	900	ADP	O4'-C4'-C5'-O5'
3	C	900	ADP	C3'-C4'-C5'-O5'
3	A	900	ADP	C5'-O5'-PA-O1A
3	A	900	ADP	O4'-C4'-C5'-O5'
3	B	900	ADP	O4'-C4'-C5'-O5'
3	A	900	ADP	C3'-C4'-C5'-O5'
3	B	900	ADP	C3'-C4'-C5'-O5'
3	D	900	ADP	O4'-C4'-C5'-O5'
3	D	900	ADP	C3'-C4'-C5'-O5'
3	B	900	ADP	PB-O3A-PA-O2A
3	D	900	ADP	PB-O3A-PA-O2A
3	B	900	ADP	C5'-O5'-PA-O1A
3	D	900	ADP	C5'-O5'-PA-O1A

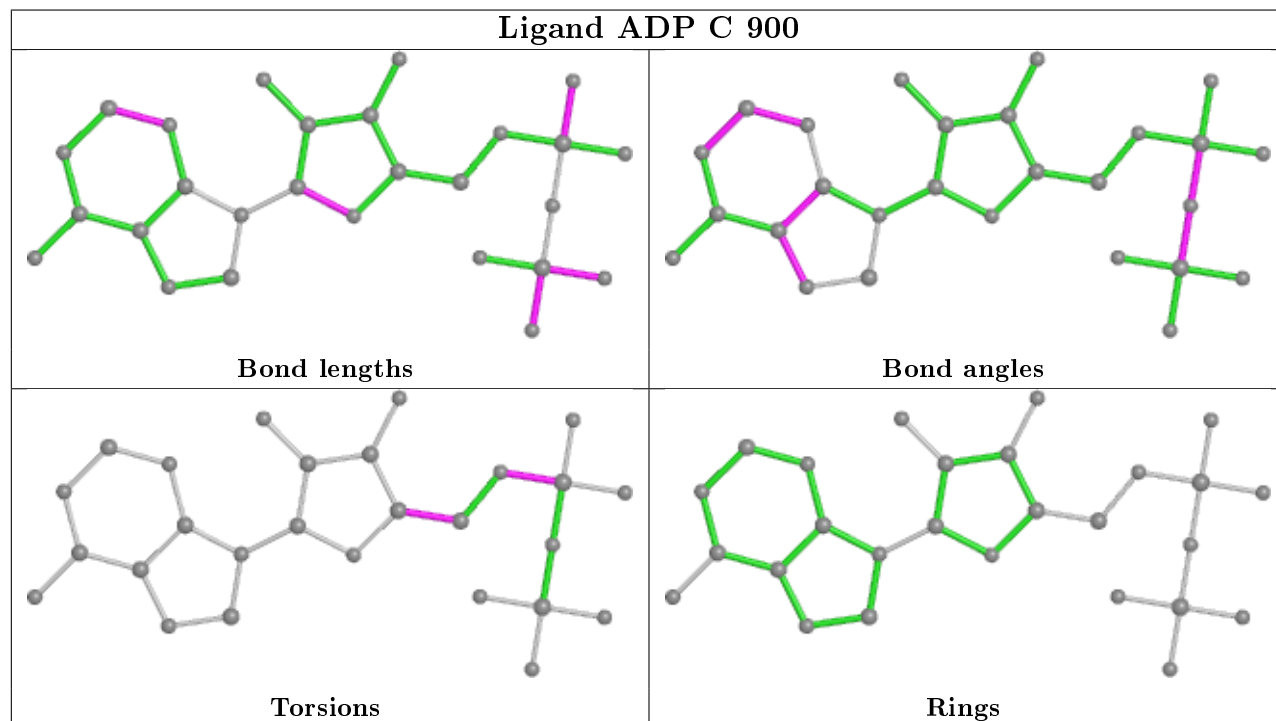
There are no ring outliers.

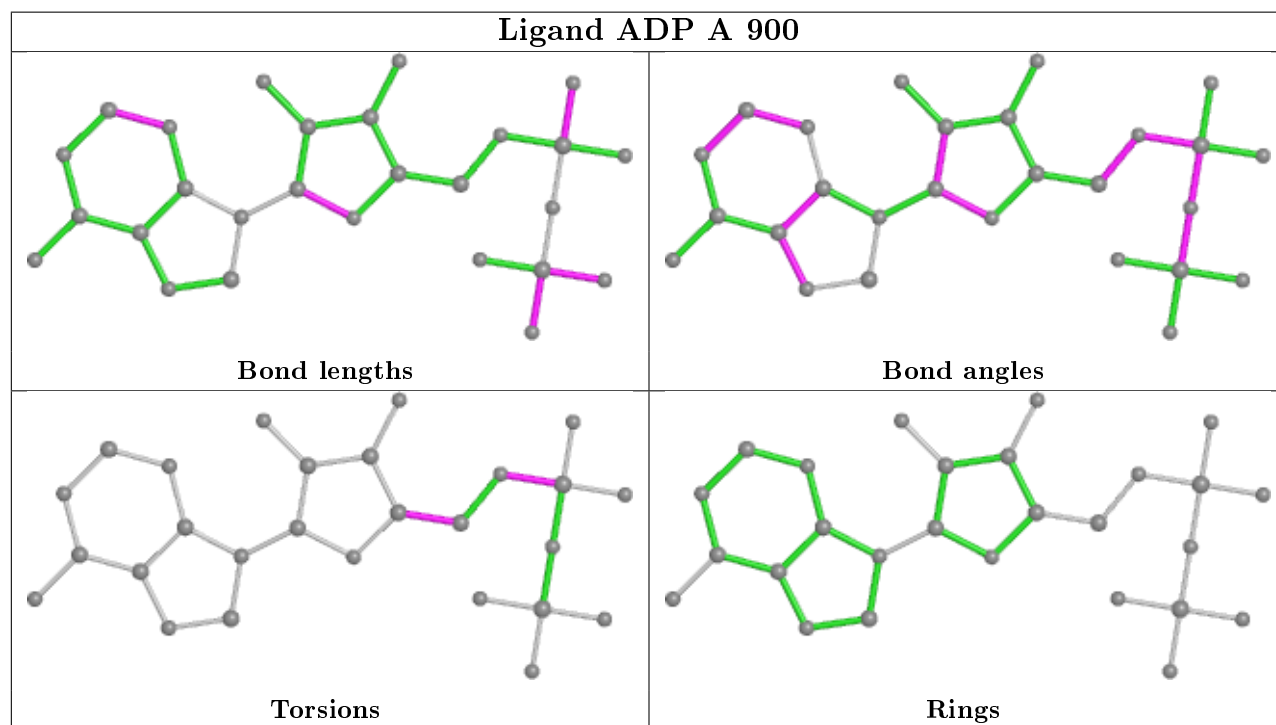
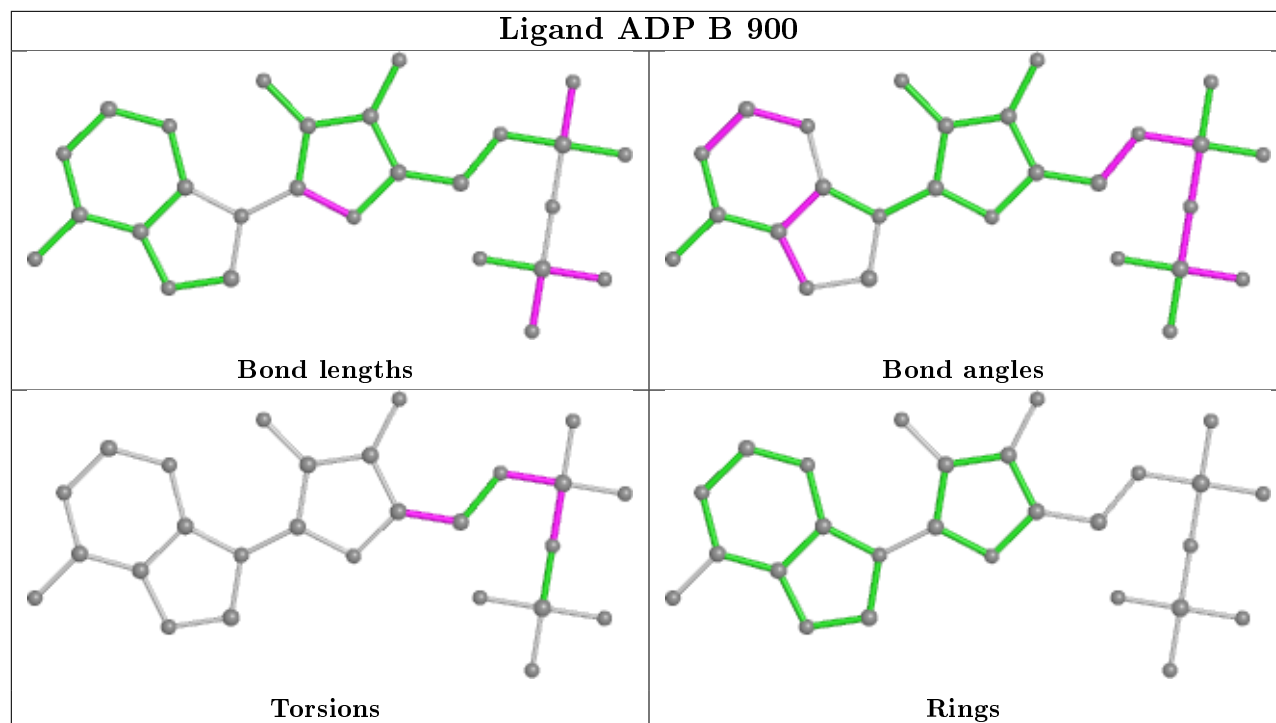
9 monomers are involved in 16 short contacts:

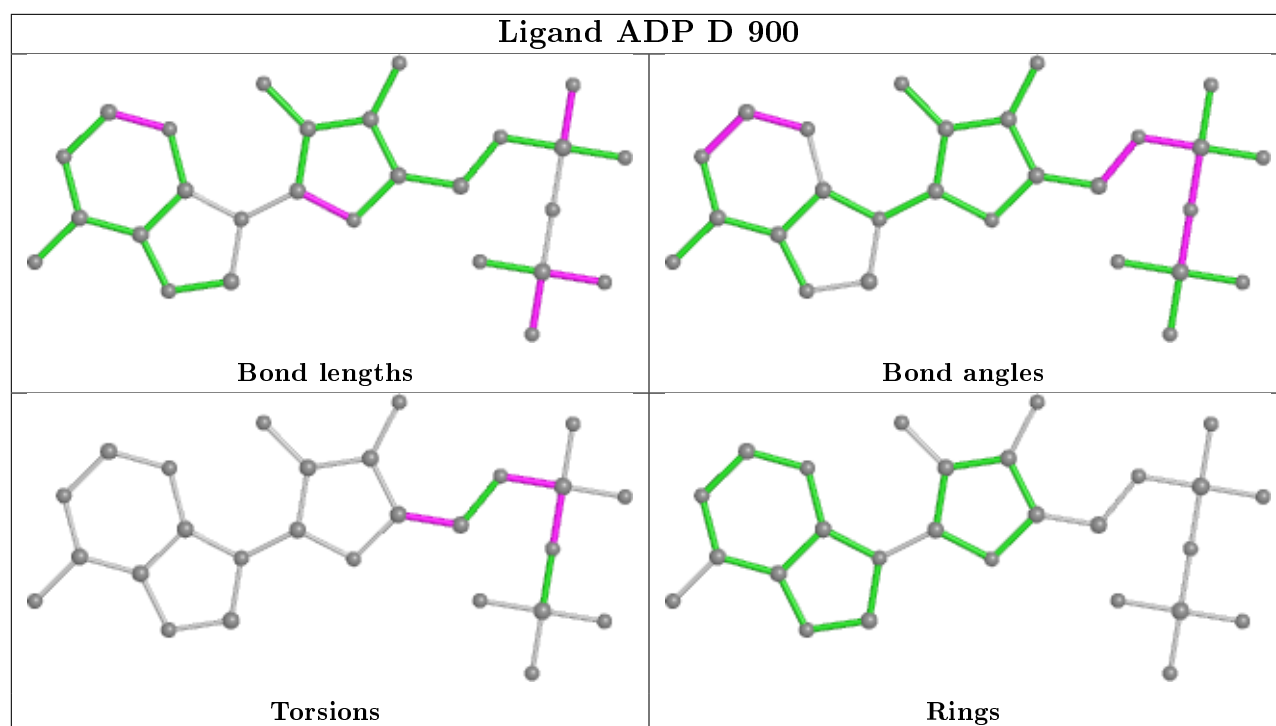
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	900	ADP	3	0
3	B	900	ADP	2	0
3	A	900	ADP	3	0
3	D	900	ADP	2	0
4	B	902	SO4	1	0
4	D	901	SO4	1	0
4	C	902	SO4	1	0
4	C	901	SO4	1	0
4	A	902	SO4	2	0

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 [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	347/356 (97%)	0.16	1 (0%) 94 92	37, 60, 87, 107	0
1	B	347/356 (97%)	0.25	3 (0%) 84 75	42, 66, 86, 119	0
1	C	347/356 (97%)	0.30	2 (0%) 89 83	45, 70, 101, 112	0
1	D	347/356 (97%)	0.30	6 (1%) 70 57	49, 72, 100, 135	0
2	E	86/133 (64%)	0.34	2 (2%) 60 47	54, 77, 108, 114	0
2	F	86/133 (64%)	0.37	2 (2%) 60 47	55, 85, 119, 152	0
2	G	86/133 (64%)	0.26	0 100 100	52, 80, 121, 135	0
2	H	80/133 (60%)	0.35	0 100 100	44, 63, 102, 117	0
All	All	1726/1956 (88%)	0.27	16 (0%) 84 75	37, 69, 102, 152	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	332	ASP	4.7
1	C	357	GLY	4.6
2	E	86	VAL	3.8
1	D	357	GLY	2.9
1	D	98	MET	2.8
1	A	332	ASP	2.8
1	B	332	ASP	2.6
2	F	82	TYR	2.6
2	E	82	TYR	2.6
1	D	332	ASP	2.5
1	D	330	LYS	2.4
2	F	37	GLU	2.3
1	D	120	HIS	2.3
1	B	333	MET	2.2
1	D	277	ARG	2.1
1	B	95	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

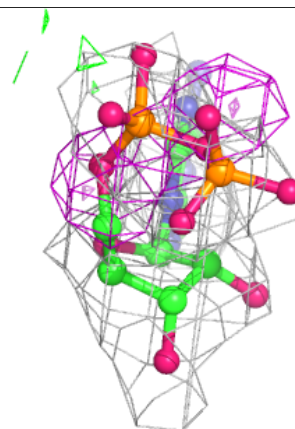
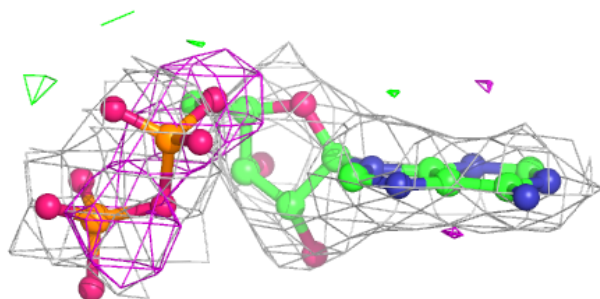
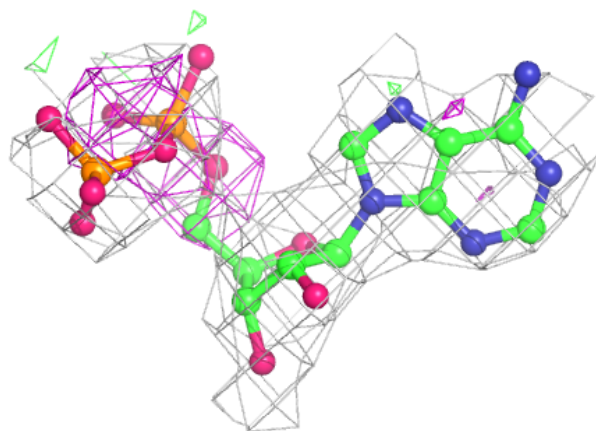
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	C	900	27/27	0.81	0.37	75,82,123,124	0
3	ADP	A	900	27/27	0.83	0.29	67,74,101,104	0
4	SO4	D	904	5/5	0.86	0.17	103,105,107,108	0
4	SO4	A	904	5/5	0.86	0.19	108,109,112,113	0
3	ADP	B	900	27/27	0.88	0.22	80,89,99,101	0
3	ADP	D	900	27/27	0.88	0.23	70,79,109,111	0
4	SO4	B	904	5/5	0.90	0.20	88,89,91,92	0
4	SO4	A	901	5/5	0.92	0.17	75,76,78,78	0
4	SO4	C	904	5/5	0.93	0.16	102,104,106,107	0
4	SO4	D	901	5/5	0.95	0.20	67,68,71,73	0
4	SO4	D	903	5/5	0.96	0.17	58,60,61,61	0
4	SO4	C	903	5/5	0.96	0.14	60,60,63,65	0
4	SO4	A	903	5/5	0.96	0.14	62,63,66,66	0
4	SO4	B	903	5/5	0.97	0.13	53,54,55,55	0
4	SO4	C	902	5/5	0.97	0.17	58,59,61,62	0
4	SO4	B	901	5/5	0.97	0.23	60,60,61,63	0
4	SO4	C	901	5/5	0.97	0.17	70,71,74,75	0
4	SO4	B	902	5/5	0.99	0.20	46,48,49,49	0
4	SO4	D	902	5/5	0.99	0.21	52,53,54,55	0
4	SO4	A	902	5/5	0.99	0.17	44,45,47,48	0

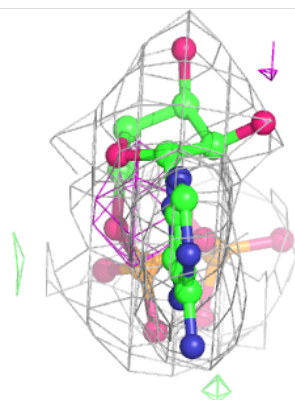
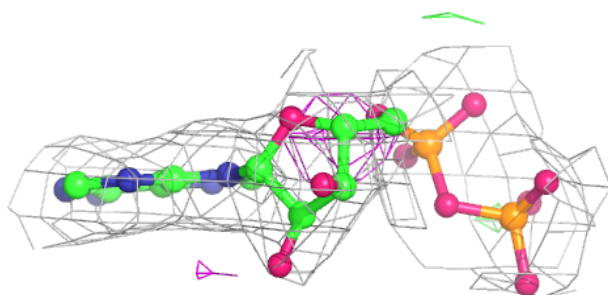
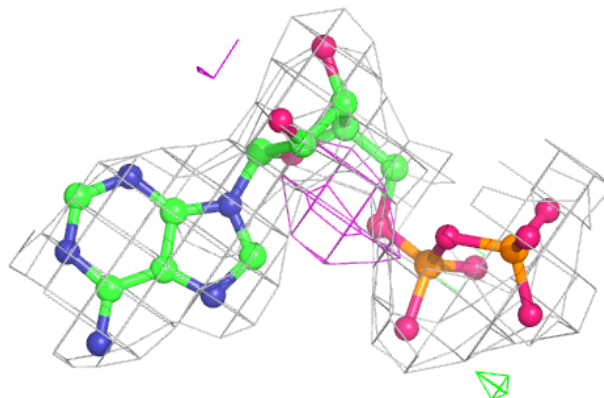
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 900:

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

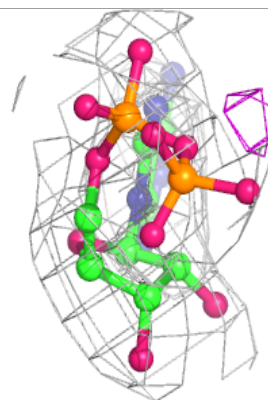
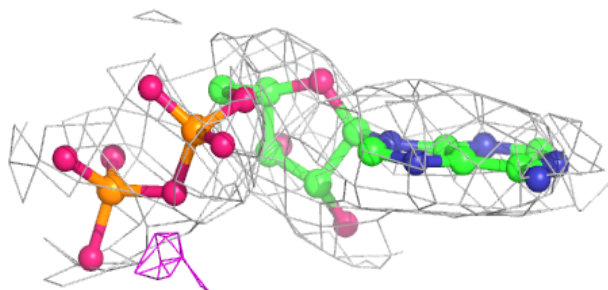
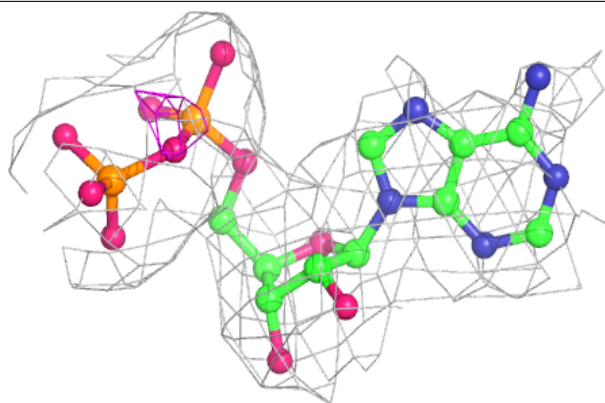
**Electron density around ADP A 900:**

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

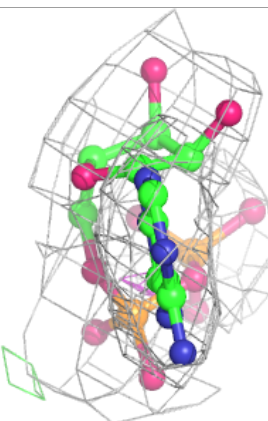
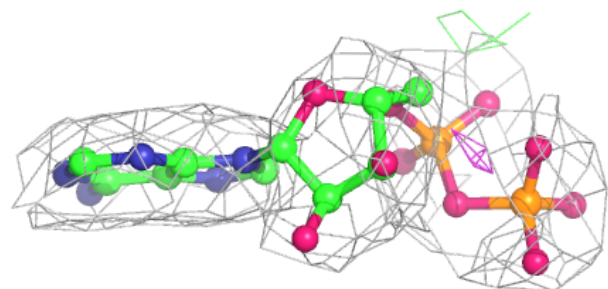
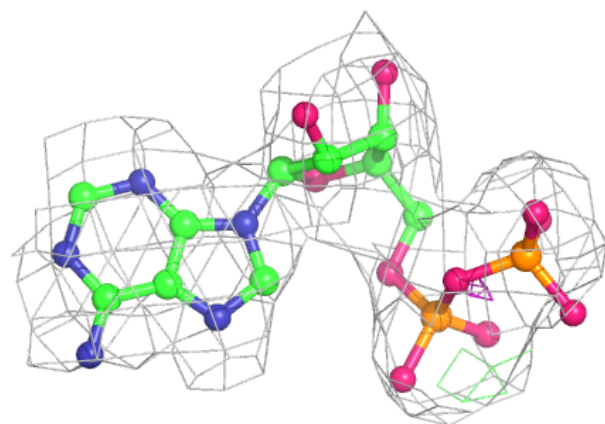


Electron density around ADP B 900:

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

**Electron density around ADP D 900:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.