Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:51 AM GMT

PDB ID	:	2OFW
Title	:	Crystal structure of the APSK domain of human PAPSS1 complexed with 2 APS molecules
Authors	:	Sekulic, N; Lavie, A
Deposited on	:	2007-01-04
Resolution	:	2.05 Å(reported)

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

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

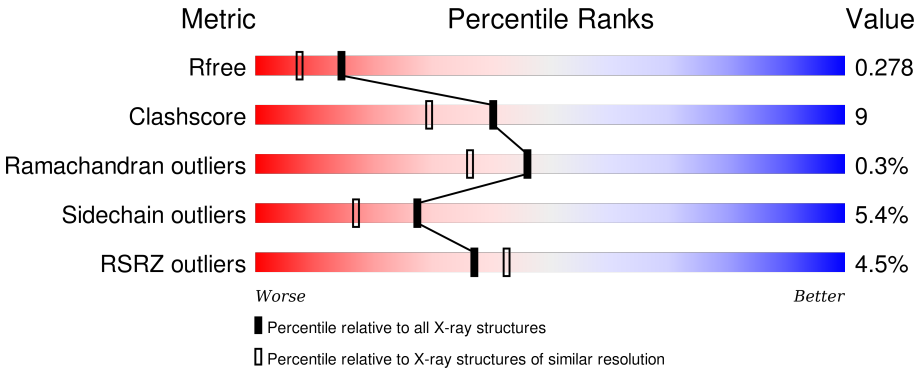
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	6% 77% 18%
1	B	208	5% 72% 18% 7%
1	C	208	2% 78% 16%
1	D	208	5% 74% 23%
1	E	208	4% 81% 13%

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Mol	Chain	Length	Quality of chain
1	F	208	5% 78% 18%
1	G	208	6% 79% 16%
1	H	208	2% 76% 15% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13687 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 APS kinase domain of the PAPS synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	3	0
			1574	979	281	306	8			
1	B	193	Total	C	N	O	S	0	0	0
			1497	935	265	289	8			
1	C	204	Total	C	N	O	S	0	0	0
			1583	987	282	306	8			
1	D	204	Total	C	N	O	S	0	0	0
			1583	987	282	306	8			
1	E	203	Total	C	N	O	S	0	0	0
			1562	974	277	303	8			
1	F	204	Total	C	N	O	S	5	0	0
			1573	981	278	306	8			
1	G	201	Total	C	N	O	S	0	0	0
			1553	971	273	301	8			
1	H	193	Total	C	N	O	S	0	0	0
			1492	932	262	290	8			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	-	CLONING ARTIFACT	UNP O43252
A	21	GLY	-	CLONING ARTIFACT	UNP O43252
A	22	HIS	-	CLONING ARTIFACT	UNP O43252
A	?	-	GLU	DELETION	UNP O43252
A	?	-	ILE	DELETION	UNP O43252
A	?	-	PRO	DELETION	UNP O43252
A	?	-	GLY	DELETION	UNP O43252
A	?	-	SER	DELETION	UNP O43252
A	?	-	LEU	DELETION	UNP O43252
A	?	-	CYS	DELETION	UNP O43252
A	?	-	LYS	DELETION	UNP O43252
A	?	-	LYS	DELETION	UNP O43252
A	?	-	VAL	DELETION	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP O43252
A	?	-	LEU	DELETION	UNP O43252
A	?	-	SER	DELETION	UNP O43252
A	?	-	ASN	DELETION	UNP O43252
A	?	-	ASN	DELETION	UNP O43252
A	?	-	ALA	DELETION	UNP O43252
A	?	-	GLN	DELETION	UNP O43252
A	?	-	ASN	DELETION	UNP O43252
A	?	-	TRP	DELETION	UNP O43252
A	?	-	GLY	DELETION	UNP O43252
A	?	-	MET	DELETION	UNP O43252
A	?	-	GLN	DELETION	UNP O43252
A	55	ILE	VAL	CONFLICT	UNP O43252
A	221	ASN	GLN	CONFLICT	UNP O43252
A	226	LEU	VAL	CONFLICT	UNP O43252
B	20	GLN	-	CLONING ARTIFACT	UNP O43252
B	21	GLY	-	CLONING ARTIFACT	UNP O43252
B	22	HIS	-	CLONING ARTIFACT	UNP O43252
B	?	-	GLU	DELETION	UNP O43252
B	?	-	ILE	DELETION	UNP O43252
B	?	-	PRO	DELETION	UNP O43252
B	?	-	GLY	DELETION	UNP O43252
B	?	-	SER	DELETION	UNP O43252
B	?	-	LEU	DELETION	UNP O43252
B	?	-	CYS	DELETION	UNP O43252
B	?	-	LYS	DELETION	UNP O43252
B	?	-	LYS	DELETION	UNP O43252
B	?	-	VAL	DELETION	UNP O43252
B	?	-	LYS	DELETION	UNP O43252
B	?	-	LEU	DELETION	UNP O43252
B	?	-	SER	DELETION	UNP O43252
B	?	-	ASN	DELETION	UNP O43252
B	?	-	ASN	DELETION	UNP O43252
B	?	-	ALA	DELETION	UNP O43252
B	?	-	GLN	DELETION	UNP O43252
B	?	-	ASN	DELETION	UNP O43252
B	?	-	TRP	DELETION	UNP O43252
B	?	-	GLY	DELETION	UNP O43252
B	?	-	MET	DELETION	UNP O43252
B	?	-	GLN	DELETION	UNP O43252
B	55	ILE	VAL	CONFLICT	UNP O43252
B	221	ASN	GLN	CONFLICT	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
B	226	LEU	VAL	CONFLICT	UNP O43252
C	20	GLN	-	CLONING ARTIFACT	UNP O43252
C	21	GLY	-	CLONING ARTIFACT	UNP O43252
C	22	HIS	-	CLONING ARTIFACT	UNP O43252
C	?	-	GLU	DELETION	UNP O43252
C	?	-	ILE	DELETION	UNP O43252
C	?	-	PRO	DELETION	UNP O43252
C	?	-	GLY	DELETION	UNP O43252
C	?	-	SER	DELETION	UNP O43252
C	?	-	LEU	DELETION	UNP O43252
C	?	-	CYS	DELETION	UNP O43252
C	?	-	LYS	DELETION	UNP O43252
C	?	-	LYS	DELETION	UNP O43252
C	?	-	VAL	DELETION	UNP O43252
C	?	-	LYS	DELETION	UNP O43252
C	?	-	LEU	DELETION	UNP O43252
C	?	-	SER	DELETION	UNP O43252
C	?	-	ASN	DELETION	UNP O43252
C	?	-	ASN	DELETION	UNP O43252
C	?	-	ALA	DELETION	UNP O43252
C	?	-	GLN	DELETION	UNP O43252
C	?	-	ASN	DELETION	UNP O43252
C	?	-	TRP	DELETION	UNP O43252
C	?	-	GLY	DELETION	UNP O43252
C	?	-	MET	DELETION	UNP O43252
C	?	-	GLN	DELETION	UNP O43252
C	55	ILE	VAL	CONFLICT	UNP O43252
C	221	ASN	GLN	CONFLICT	UNP O43252
C	226	LEU	VAL	CONFLICT	UNP O43252
D	20	GLN	-	CLONING ARTIFACT	UNP O43252
D	21	GLY	-	CLONING ARTIFACT	UNP O43252
D	22	HIS	-	CLONING ARTIFACT	UNP O43252
D	?	-	GLU	DELETION	UNP O43252
D	?	-	ILE	DELETION	UNP O43252
D	?	-	PRO	DELETION	UNP O43252
D	?	-	GLY	DELETION	UNP O43252
D	?	-	SER	DELETION	UNP O43252
D	?	-	LEU	DELETION	UNP O43252
D	?	-	CYS	DELETION	UNP O43252
D	?	-	LYS	DELETION	UNP O43252
D	?	-	LYS	DELETION	UNP O43252
D	?	-	VAL	DELETION	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LYS	DELETION	UNP O43252
D	?	-	LEU	DELETION	UNP O43252
D	?	-	SER	DELETION	UNP O43252
D	?	-	ASN	DELETION	UNP O43252
D	?	-	ASN	DELETION	UNP O43252
D	?	-	ALA	DELETION	UNP O43252
D	?	-	GLN	DELETION	UNP O43252
D	?	-	ASN	DELETION	UNP O43252
D	?	-	TRP	DELETION	UNP O43252
D	?	-	GLY	DELETION	UNP O43252
D	?	-	MET	DELETION	UNP O43252
D	?	-	GLN	DELETION	UNP O43252
D	55	ILE	VAL	CONFLICT	UNP O43252
D	221	ASN	GLN	CONFLICT	UNP O43252
D	226	LEU	VAL	CONFLICT	UNP O43252
E	20	GLN	-	CLONING ARTIFACT	UNP O43252
E	21	GLY	-	CLONING ARTIFACT	UNP O43252
E	22	HIS	-	CLONING ARTIFACT	UNP O43252
E	?	-	GLU	DELETION	UNP O43252
E	?	-	ILE	DELETION	UNP O43252
E	?	-	PRO	DELETION	UNP O43252
E	?	-	GLY	DELETION	UNP O43252
E	?	-	SER	DELETION	UNP O43252
E	?	-	LEU	DELETION	UNP O43252
E	?	-	CYS	DELETION	UNP O43252
E	?	-	LYS	DELETION	UNP O43252
E	?	-	LYS	DELETION	UNP O43252
E	?	-	VAL	DELETION	UNP O43252
E	?	-	LYS	DELETION	UNP O43252
E	?	-	LEU	DELETION	UNP O43252
E	?	-	SER	DELETION	UNP O43252
E	?	-	ASN	DELETION	UNP O43252
E	?	-	ASN	DELETION	UNP O43252
E	?	-	ALA	DELETION	UNP O43252
E	?	-	GLN	DELETION	UNP O43252
E	?	-	ASN	DELETION	UNP O43252
E	?	-	TRP	DELETION	UNP O43252
E	?	-	GLY	DELETION	UNP O43252
E	?	-	MET	DELETION	UNP O43252
E	?	-	GLN	DELETION	UNP O43252
E	55	ILE	VAL	CONFLICT	UNP O43252
E	221	ASN	GLN	CONFLICT	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
E	226	LEU	VAL	CONFLICT	UNP O43252
F	20	GLN	-	CLONING ARTIFACT	UNP O43252
F	21	GLY	-	CLONING ARTIFACT	UNP O43252
F	22	HIS	-	CLONING ARTIFACT	UNP O43252
F	?	-	GLU	DELETION	UNP O43252
F	?	-	ILE	DELETION	UNP O43252
F	?	-	PRO	DELETION	UNP O43252
F	?	-	GLY	DELETION	UNP O43252
F	?	-	SER	DELETION	UNP O43252
F	?	-	LEU	DELETION	UNP O43252
F	?	-	CYS	DELETION	UNP O43252
F	?	-	LYS	DELETION	UNP O43252
F	?	-	LYS	DELETION	UNP O43252
F	?	-	VAL	DELETION	UNP O43252
F	?	-	LYS	DELETION	UNP O43252
F	?	-	LEU	DELETION	UNP O43252
F	?	-	SER	DELETION	UNP O43252
F	?	-	ASN	DELETION	UNP O43252
F	?	-	ASN	DELETION	UNP O43252
F	?	-	ALA	DELETION	UNP O43252
F	?	-	GLN	DELETION	UNP O43252
F	?	-	ASN	DELETION	UNP O43252
F	?	-	TRP	DELETION	UNP O43252
F	?	-	GLY	DELETION	UNP O43252
F	?	-	MET	DELETION	UNP O43252
F	?	-	GLN	DELETION	UNP O43252
F	55	ILE	VAL	CONFLICT	UNP O43252
F	221	ASN	GLN	CONFLICT	UNP O43252
F	226	LEU	VAL	CONFLICT	UNP O43252
G	20	GLN	-	CLONING ARTIFACT	UNP O43252
G	21	GLY	-	CLONING ARTIFACT	UNP O43252
G	22	HIS	-	CLONING ARTIFACT	UNP O43252
G	?	-	GLU	DELETION	UNP O43252
G	?	-	ILE	DELETION	UNP O43252
G	?	-	PRO	DELETION	UNP O43252
G	?	-	GLY	DELETION	UNP O43252
G	?	-	SER	DELETION	UNP O43252
G	?	-	LEU	DELETION	UNP O43252
G	?	-	CYS	DELETION	UNP O43252
G	?	-	LYS	DELETION	UNP O43252
G	?	-	LYS	DELETION	UNP O43252
G	?	-	VAL	DELETION	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	DELETION	UNP O43252
G	?	-	LEU	DELETION	UNP O43252
G	?	-	SER	DELETION	UNP O43252
G	?	-	ASN	DELETION	UNP O43252
G	?	-	ASN	DELETION	UNP O43252
G	?	-	ALA	DELETION	UNP O43252
G	?	-	GLN	DELETION	UNP O43252
G	?	-	ASN	DELETION	UNP O43252
G	?	-	TRP	DELETION	UNP O43252
G	?	-	GLY	DELETION	UNP O43252
G	?	-	MET	DELETION	UNP O43252
G	?	-	GLN	DELETION	UNP O43252
G	55	ILE	VAL	CONFLICT	UNP O43252
G	221	ASN	GLN	CONFLICT	UNP O43252
G	226	LEU	VAL	CONFLICT	UNP O43252
H	20	GLN	-	CLONING ARTIFACT	UNP O43252
H	21	GLY	-	CLONING ARTIFACT	UNP O43252
H	22	HIS	-	CLONING ARTIFACT	UNP O43252
H	?	-	GLU	DELETION	UNP O43252
H	?	-	ILE	DELETION	UNP O43252
H	?	-	PRO	DELETION	UNP O43252
H	?	-	GLY	DELETION	UNP O43252
H	?	-	SER	DELETION	UNP O43252
H	?	-	LEU	DELETION	UNP O43252
H	?	-	CYS	DELETION	UNP O43252
H	?	-	LYS	DELETION	UNP O43252
H	?	-	LYS	DELETION	UNP O43252
H	?	-	VAL	DELETION	UNP O43252
H	?	-	LYS	DELETION	UNP O43252
H	?	-	LEU	DELETION	UNP O43252
H	?	-	SER	DELETION	UNP O43252
H	?	-	ASN	DELETION	UNP O43252
H	?	-	ASN	DELETION	UNP O43252
H	?	-	ALA	DELETION	UNP O43252
H	?	-	GLN	DELETION	UNP O43252
H	?	-	ASN	DELETION	UNP O43252
H	?	-	TRP	DELETION	UNP O43252
H	?	-	GLY	DELETION	UNP O43252
H	?	-	MET	DELETION	UNP O43252
H	?	-	GLN	DELETION	UNP O43252
H	55	ILE	VAL	CONFLICT	UNP O43252
H	221	ASN	GLN	CONFLICT	UNP O43252

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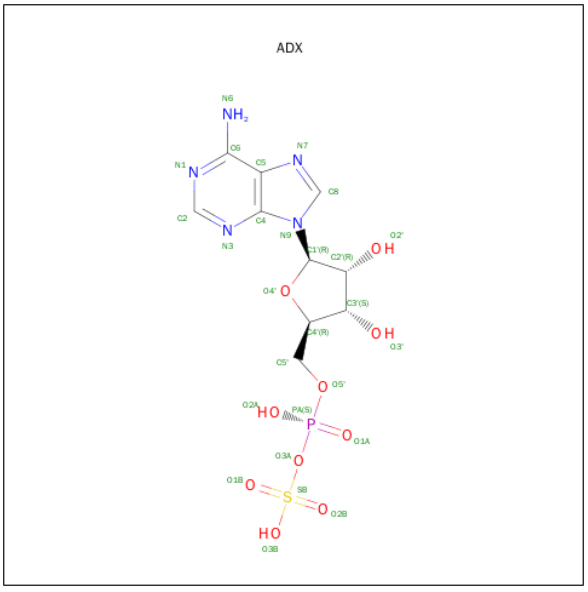
Chain	Residue	Modelled	Actual	Comment	Reference
H	226	LEU	VAL	CONFLICT	UNP O43252

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	F	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	G	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	H	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	A	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	F	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	G	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	H	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	104	Total	O	0	0
			104	104		
4	C	108	Total	O	0	0
			108	108		
4	D	103	Total	O	0	0
			103	103		
4	E	103	Total	O	0	0
			103	103		

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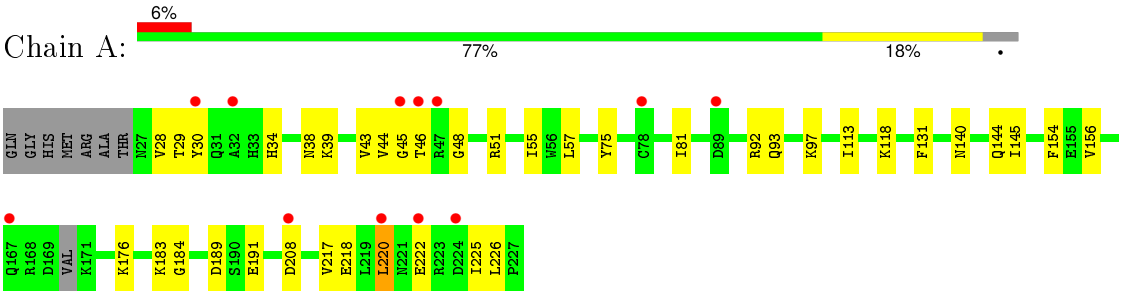
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	92	Total O 92 92	0	0
4	G	103	Total O 103 103	0	0
4	H	102	Total O 102 102	0	0

3 Residue-property plots (i)

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

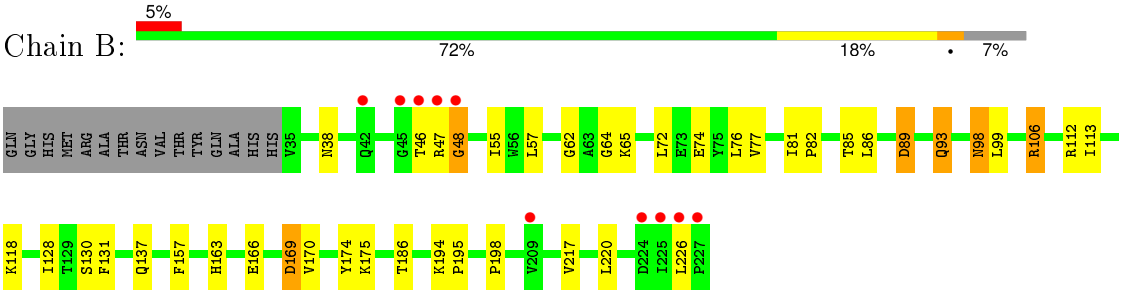
- Molecule 1: APS kinase domain of the PAPS synthetase 1

Chain A:



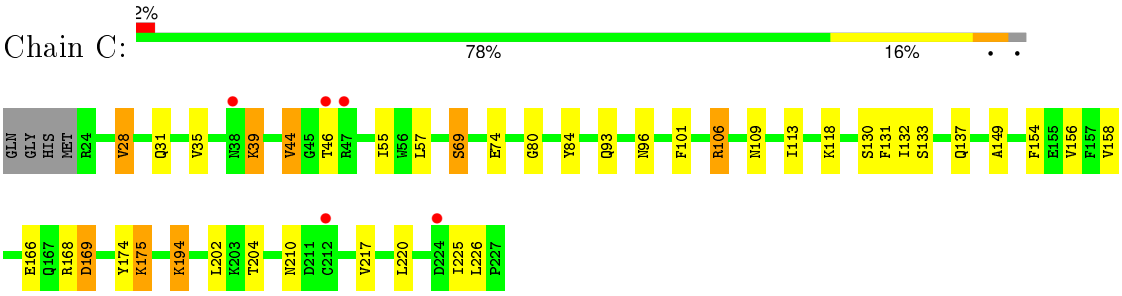
- Molecule 1: APS kinase domain of the PAPS synthetase 1

Chain B:



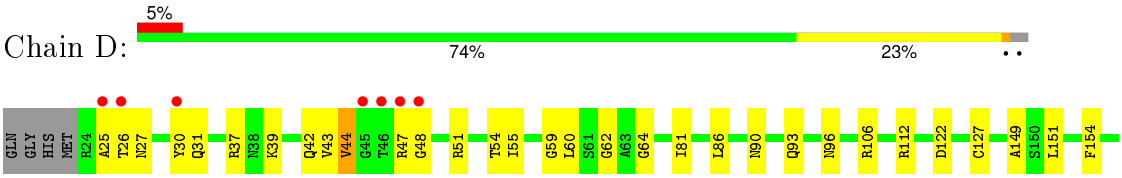
- Molecule 1: APS kinase domain of the PAPS synthetase 1

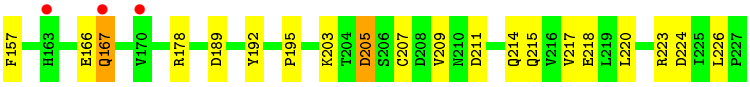
Chain C:



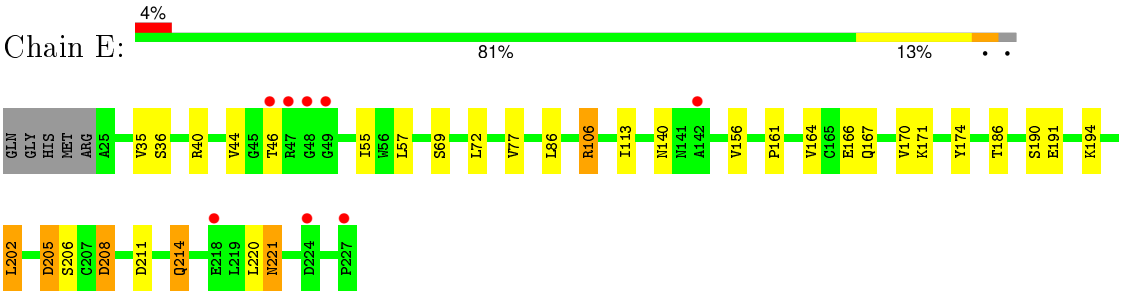
- Molecule 1: APS kinase domain of the PAPS synthetase 1

Chain D:

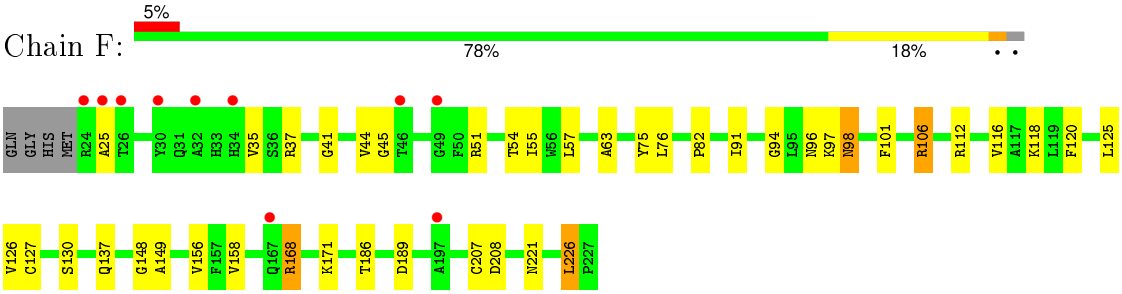




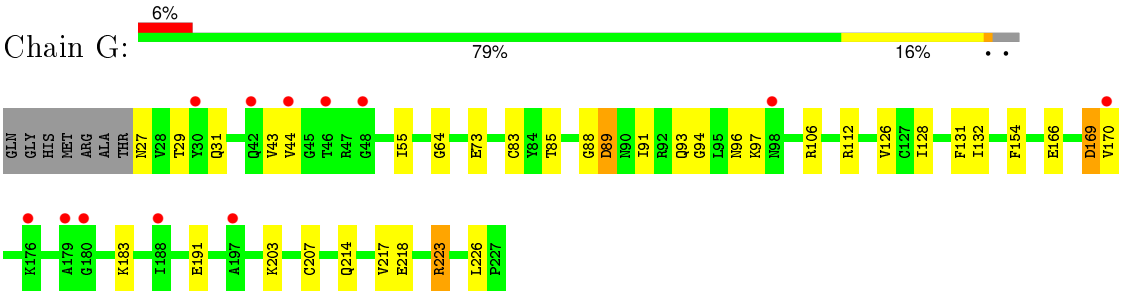
• Molecule 1: APS kinase domain of the PAPS synthetase 1



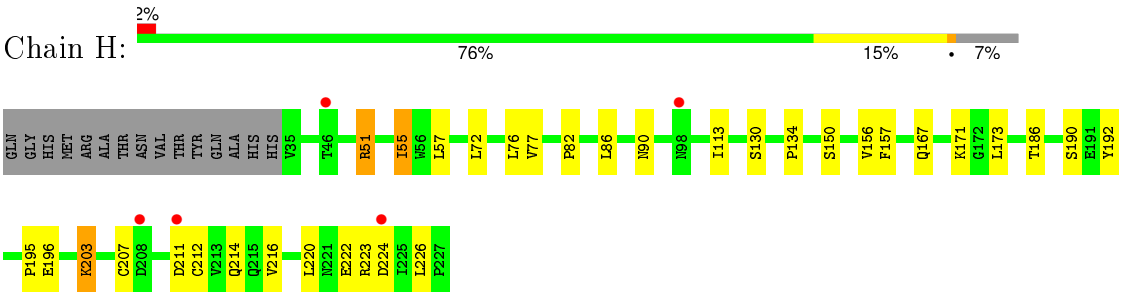
• Molecule 1: APS kinase domain of the PAPS synthetase 1



• Molecule 1: APS kinase domain of the PAPS synthetase 1



• Molecule 1: APS kinase domain of the PAPS synthetase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.19Å 69.03Å 150.61Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 15.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-2.05) 97.4 (15.00-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.12 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.282 0.216 , 0.278	Depositor DCC
R_{free} test set	10107 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	1 of 101697 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13687	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADX

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	0.56	0/1601	0.66	0/2165
1	B	0.58	0/1522	0.69	2/2057 (0.1%)
1	C	0.57	0/1611	0.69	2/2179 (0.1%)
1	D	0.58	0/1611	0.65	0/2179
1	E	0.55	0/1590	0.69	2/2153 (0.1%)
1	F	0.55	0/1601	0.68	2/2168 (0.1%)
1	G	0.57	0/1581	0.69	2/2141 (0.1%)
1	H	0.55	0/1517	0.64	0/2050
All	All	0.56	0/12634	0.67	10/17092 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	106	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	E	106	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	C	106	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	F	106	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	E	106	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	F	106	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	G	106	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	G	106	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	106	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	106	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1574	0	1528	25	0
1	B	1497	0	1478	38	0
1	C	1583	0	1550	32	0
1	D	1583	0	1550	44	0
1	E	1562	0	1516	19	0
1	F	1573	0	1528	31	0
1	G	1553	0	1515	27	0
1	H	1492	0	1467	24	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
3	A	54	0	24	0	0
3	B	54	0	24	2	0
3	C	54	0	26	3	0
3	D	54	0	24	3	0
3	E	54	0	25	1	0
3	F	54	0	25	2	0
3	G	54	0	25	3	0
3	H	54	0	25	0	0
4	A	117	0	0	3	1
4	B	104	0	0	5	0
4	C	108	0	0	2	1
4	D	103	0	0	9	0
4	E	103	0	0	2	0
4	F	92	0	0	1	0
4	G	103	0	0	0	0
4	H	102	0	0	1	0
All	All	13687	0	12330	219	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (219) 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)
4:C:1407:HOH:O	1:D:25:ALA:HB2	1.44	1.14
1:C:31:GLN:H	1:D:90:ASN:HD21	1.15	0.94
1:C:44:VAL:O	1:D:44:VAL:O	1.84	0.94
1:B:175:LYS:HD2	4:B:1234:HOH:O	1.78	0.83
1:D:55:ILE:HD11	1:D:220:LEU:HD11	1.63	0.80
4:E:1564:HOH:O	1:F:25:ALA:HB2	1.82	0.78
1:D:214:GLN:O	1:D:218:GLU:HG2	1.83	0.76
1:D:106:ARG:NE	4:D:1502:HOH:O	2.12	0.74
1:A:29:THR:N	1:B:89:ASP:OD1	2.21	0.73
1:A:220:LEU:HB3	1:A:226:LEU:HG	1.70	0.72
1:F:98:ASN:HD21	1:F:112:ARG:HH12	1.35	0.72
1:A:44:VAL:HG12	1:B:82:PRO:HB3	1.71	0.71
1:H:186:THR:HA	1:H:190:SER:HB3	1.71	0.71
1:H:220:LEU:HB3	1:H:226:LEU:HD13	1.73	0.71
1:D:166:GLU:OE1	1:D:178:ARG:NH2	2.24	0.70
1:D:62:GLY:O	3:D:1401:ADX:H5"	1.92	0.70
1:G:31:GLN:H	1:H:90:ASN:HD21	1.40	0.69
1:A:140:ASN:O	1:A:144:GLN:HG3	1.92	0.69
1:F:120:PHE:HD1	1:F:125:LEU:HD12	1.58	0.68
1:C:217:VAL:HG13	1:C:226:LEU:CD2	2.24	0.68
1:A:55:ILE:CD1	1:A:154:PHE:HD1	2.07	0.68
1:G:94:GLY:O	1:G:97:LYS:HG2	1.95	0.67
1:B:98:ASN:HD22	1:B:98:ASN:H	1.41	0.67
1:B:217:VAL:HG13	1:B:226:LEU:HD23	1.77	0.66
1:C:168:ARG:HH22	1:C:204:THR:HG22	1.61	0.66
1:H:57:LEU:HD23	1:H:156:VAL:HB	1.76	0.66
1:G:214:GLN:O	1:G:218:GLU:HG2	1.96	0.66
1:D:37:ARG:NH1	1:D:122:ASP:OD1	2.29	0.66
1:A:113:ILE:HG12	1:A:131:PHE:CZ	2.31	0.65
1:B:57:LEU:HD12	1:B:130:SER:HB3	1.78	0.65
1:H:72:LEU:O	1:H:76:LEU:HD23	1.97	0.64
1:C:101:PHE:O	1:C:106:ARG:HD2	1.98	0.64
1:A:43:VAL:HG21	1:B:77:VAL:HG13	1.79	0.64
1:H:55:ILE:HD11	1:H:220:LEU:HD21	1.78	0.64
1:E:170:VAL:HG23	1:E:171:LYS:HG3	1.79	0.64
1:F:189:ASP:O	4:F:1616:HOH:O	2.15	0.64
1:C:217:VAL:HG13	1:C:226:LEU:HD22	1.80	0.64
1:D:154:PHE:CE2	1:D:223:ARG:HG3	2.33	0.64
1:G:89:ASP:HA	1:G:93:GLN:HE22	1.62	0.64
1:G:217:VAL:HG13	1:G:226:LEU:HD23	1.81	0.63
1:F:76:LEU:HD22	1:F:226:LEU:HD21	1.79	0.63
1:A:57:LEU:HD23	1:A:156:VAL:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:HD23	1:C:156:VAL:HB	1.82	0.61
1:B:65:LYS:HB3	1:B:130:SER:HB2	1.83	0.60
1:B:98:ASN:HD21	1:B:112:ARG:HH12	1.47	0.60
1:B:98:ASN:ND2	1:B:98:ASN:H	1.99	0.60
1:C:118:LYS:HE3	1:C:149:ALA:HB2	1.83	0.60
1:F:51:ARG:HH21	1:F:82:PRO:HD2	1.66	0.60
1:D:37:ARG:NH1	1:D:151:LEU:HD21	2.17	0.59
1:C:80:GLY:HA2	1:D:43:VAL:HG23	1.84	0.59
1:F:76:LEU:CD2	1:F:226:LEU:HD21	2.34	0.58
1:D:106:ARG:NH2	4:D:1502:HOH:O	2.36	0.58
1:C:204:THR:HG23	3:C:1301:ADX:C6	2.34	0.58
1:D:93:GLN:NE2	4:D:1477:HOH:O	2.36	0.58
1:B:166:GLU:HG2	1:B:174:TYR:CD1	2.40	0.57
1:G:31:GLN:N	1:H:90:ASN:HD21	2.03	0.57
1:C:55:ILE:HD11	1:C:220:LEU:HD21	1.87	0.57
1:A:154:PHE:CZ	1:A:225:ILE:HD11	2.39	0.57
1:B:93:GLN:HE21	1:B:93:GLN:HA	1.70	0.56
1:H:86:LEU:HD13	1:H:113:ILE:HD11	1.87	0.56
1:C:55:ILE:CD1	1:C:220:LEU:HD21	2.36	0.56
1:A:34:HIS:HB2	4:B:1305:HOH:O	2.07	0.56
1:C:93:GLN:HE22	1:D:30:TYR:HB2	1.71	0.55
1:H:76:LEU:HD11	1:H:226:LEU:HD11	1.87	0.55
1:G:55:ILE:HD11	1:G:126:VAL:HG13	1.89	0.55
1:E:44:VAL:O	1:F:44:VAL:O	2.25	0.54
1:C:113:ILE:HG12	1:C:131:PHE:CZ	2.42	0.54
1:F:51:ARG:HG3	1:F:51:ARG:HH11	1.73	0.54
1:G:64:GLY:HA2	3:G:1701:ADX:H5"	1.89	0.54
1:G:64:GLY:HA2	3:G:1701:ADX:C5'	2.37	0.54
1:A:81:ILE:HD13	1:A:226:LEU:HD22	1.90	0.53
1:A:55:ILE:CD1	1:A:154:PHE:CD1	2.91	0.53
1:F:106:ARG:NH2	1:F:186:THR:OG1	2.42	0.53
1:D:106:ARG:CZ	4:D:1502:HOH:O	2.55	0.53
1:D:167:GLN:O	1:D:167:GLN:HG3	2.08	0.53
1:E:55:ILE:HD11	1:E:220:LEU:HD11	1.91	0.52
1:B:195:PRO:HB2	1:B:198:PRO:HD3	1.91	0.52
1:G:27:ASN:HB3	1:H:173:LEU:HD21	1.91	0.52
1:F:120:PHE:CD1	1:F:125:LEU:HD12	2.43	0.52
1:A:140:ASN:OD1	4:A:1111:HOH:O	2.19	0.52
1:D:207:CYS:O	3:D:1401:ADX:N6	2.41	0.52
1:E:156:VAL:CG1	1:E:202:LEU:HD22	2.40	0.52
1:E:36:SER:O	1:E:40:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ILE:CD1	1:G:126:VAL:HG13	2.40	0.52
1:D:154:PHE:HE2	1:D:223:ARG:HG3	1.75	0.51
1:B:38:ASN:ND2	1:B:38:ASN:H	2.08	0.51
1:D:106:ARG:NH1	4:D:1461:HOH:O	2.42	0.51
1:F:91:ILE:HG22	1:F:96:ASN:HB2	1.91	0.51
1:D:93:GLN:HE22	1:F:171:LYS:HA	1.75	0.51
1:C:166:GLU:HG3	1:C:174:TYR:HB3	1.92	0.51
1:F:221:ASN:OD1	1:F:226:LEU:HB3	2.10	0.51
1:B:76:LEU:CD2	1:B:226:LEU:HD11	2.40	0.50
1:C:204:THR:HG23	3:C:1301:ADX:C5	2.41	0.50
1:F:112:ARG:O	1:F:116:VAL:HG23	2.12	0.50
1:D:55:ILE:CD1	1:D:220:LEU:HD11	2.39	0.50
1:F:51:ARG:NH2	1:F:82:PRO:HD2	2.26	0.50
1:D:211:ASP:O	1:D:215:GLN:HG3	2.12	0.49
1:G:154:PHE:CE2	1:G:223:ARG:HG2	2.46	0.49
1:E:86:LEU:HD13	1:E:113:ILE:HD11	1.94	0.49
1:H:223:ARG:O	1:H:224:ASP:HB2	2.11	0.49
1:F:96:ASN:OD1	1:F:112:ARG:HD2	2.13	0.49
1:B:86:LEU:HD13	1:B:113:ILE:HD11	1.95	0.49
1:G:88:GLY:O	1:G:93:GLN:NE2	2.46	0.48
1:B:217:VAL:HG13	1:B:226:LEU:CD2	2.41	0.48
1:E:106:ARG:NH2	1:E:186:THR:OG1	2.46	0.48
1:G:166:GLU:O	1:G:169:ASP:HB2	2.14	0.48
1:A:44:VAL:HG23	1:A:45:GLY:N	2.29	0.48
1:E:57:LEU:HD23	1:E:156:VAL:HB	1.96	0.48
1:B:113:ILE:HG12	1:B:131:PHE:CZ	2.49	0.48
1:D:207:CYS:SG	1:D:211:ASP:HB3	2.54	0.48
1:G:31:GLN:H	1:H:90:ASN:ND2	2.08	0.47
1:G:154:PHE:HE2	1:G:223:ARG:HG2	1.78	0.47
1:F:37:ARG:NH2	1:F:149:ALA:O	2.39	0.47
1:F:94:GLY:O	1:F:97:LYS:HG2	2.14	0.47
1:A:191:GLU:HG2	4:A:1195:HOH:O	2.14	0.47
1:E:140:ASN:HD22	1:E:140:ASN:N	2.11	0.47
1:E:166:GLU:HG3	1:E:174:TYR:HB3	1.95	0.47
1:B:98:ASN:HD22	1:B:98:ASN:N	2.05	0.47
1:G:55:ILE:N	1:G:55:ILE:HD12	2.29	0.47
1:E:55:ILE:HD13	1:E:72:LEU:HD21	1.96	0.46
1:C:158:VAL:HG22	1:C:202:LEU:HD12	1.97	0.46
1:E:208:ASP:OD2	1:E:211:ASP:HB2	2.14	0.46
1:H:55:ILE:HD12	1:H:72:LEU:HD21	1.97	0.46
1:D:106:ARG:NH1	4:D:1479:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ILE:CD1	1:G:126:VAL:CG1	2.94	0.46
1:F:168:ARG:HD3	3:F:1601:ADX:O4'	2.16	0.46
1:B:157:PHE:CZ	1:B:194:LYS:HG2	2.51	0.45
1:C:220:LEU:HB3	1:C:225:ILE:HB	1.98	0.45
1:D:209:VAL:HG23	4:D:1450:HOH:O	2.16	0.45
1:B:98:ASN:N	1:B:98:ASN:ND2	2.65	0.45
1:F:207:CYS:O	3:F:1601:ADX:N6	2.50	0.45
1:H:134:PRO:HA	1:H:192:TYR:CD1	2.52	0.45
1:B:64:GLY:HA2	3:B:1201:ADX:H5'	1.99	0.45
1:F:63:ALA:HB1	1:F:158:VAL:HG12	1.99	0.45
1:B:166:GLU:O	1:B:169:ASP:HB2	2.16	0.44
1:D:39:LYS:O	1:D:42:GLN:HG2	2.17	0.44
1:F:54:THR:HA	1:F:127:CYS:O	2.17	0.44
1:F:55:ILE:CD1	1:F:126:VAL:HG13	2.47	0.44
1:B:89:ASP:OD2	4:B:1261:HOH:O	2.21	0.44
1:D:64:GLY:HA2	3:D:1401:ADX:H5'	1.98	0.44
1:A:39:LYS:O	1:A:43:VAL:HG23	2.17	0.44
1:F:101:PHE:O	1:F:106:ARG:HD2	2.17	0.44
1:G:44:VAL:HG12	1:H:82:PRO:HB3	1.99	0.44
1:B:38:ASN:H	1:B:38:ASN:HD22	1.66	0.44
1:G:132:ILE:HD12	3:G:1700:ADX:H5'	1.99	0.44
1:G:85:THR:HG22	1:G:128:ILE:HB	1.99	0.44
1:A:28:VAL:HG13	1:B:89:ASP:CG	2.38	0.44
1:C:28:VAL:HG22	4:D:1477:HOH:O	2.16	0.44
1:B:62:GLY:O	3:B:1201:ADX:H5"	2.18	0.44
1:H:212:CYS:O	1:H:216:VAL:HG23	2.18	0.44
1:D:59:GLY:HA2	1:D:192:TYR:CZ	2.53	0.44
1:D:203:LYS:O	1:D:207:CYS:HB3	2.18	0.44
1:C:84:TYR:OH	1:D:122:ASP:OD2	2.23	0.44
1:H:157:PHE:HB2	1:H:195:PRO:HG2	2.00	0.44
1:F:41:GLY:HA2	1:F:44:VAL:HG12	2.00	0.44
1:F:57:LEU:HD23	1:F:156:VAL:HB	1.99	0.44
1:E:161:PRO:HG2	1:E:164:VAL:HG23	1.99	0.43
1:H:220:LEU:HD13	1:H:226:LEU:CD1	2.48	0.43
1:D:31:GLN:NE2	4:D:1402:HOH:O	2.40	0.43
1:C:96:ASN:HD22	1:C:109:ASN:ND2	2.16	0.43
1:C:210:ASN:ND2	4:C:1366:HOH:O	2.46	0.43
3:C:1300:ADX:H1'	1:D:27:ASN:O	2.18	0.43
1:A:29:THR:O	1:B:89:ASP:OD1	2.37	0.43
1:B:81:ILE:HA	1:B:82:PRO:HD3	1.88	0.43
1:D:157:PHE:HB2	1:D:195:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LEU:CD1	1:E:69:SER:HB3	2.48	0.43
1:E:214:GLN:NE2	4:E:1517:HOH:O	2.50	0.43
1:H:55:ILE:CD1	1:H:220:LEU:HD21	2.48	0.43
1:A:75:TYR:C	1:A:75:TYR:CD2	2.91	0.43
1:D:214:GLN:O	1:D:218:GLU:CG	2.62	0.43
1:A:184:GLY:HA2	1:A:189:ASP:HB3	1.99	0.43
1:A:154:PHE:HZ	1:A:225:ILE:HD11	1.84	0.43
1:H:51:ARG:HD3	4:H:1845:HOH:O	2.19	0.43
1:D:86:LEU:HD12	1:D:127:CYS:SG	2.58	0.43
1:G:43:VAL:HG21	1:H:77:VAL:O	2.19	0.42
1:D:48:GLY:O	1:D:51:ARG:NH2	2.53	0.42
1:H:51:ARG:HH21	1:H:82:PRO:CD	2.33	0.42
1:C:168:ARG:O	1:C:169:ASP:C	2.58	0.42
1:A:51:ARG:HB2	1:A:225:ILE:HG23	2.02	0.42
1:B:55:ILE:HD11	1:B:220:LEU:HD11	2.02	0.42
1:F:148:GLY:O	1:G:29:THR:HG21	2.19	0.42
1:C:166:GLU:O	1:C:169:ASP:HB2	2.19	0.42
1:B:47:ARG:O	1:B:48:GLY:O	2.37	0.42
1:D:205:ASP:N	1:D:205:ASP:OD1	2.49	0.42
1:G:73:GLU:HG3	1:G:83:CYS:SG	2.60	0.42
1:C:113:ILE:HA	1:C:113:ILE:HD12	1.94	0.41
1:G:96:ASN:OD1	1:G:112:ARG:HD2	2.20	0.41
1:D:220:LEU:HB2	1:D:226:LEU:HD22	2.02	0.41
1:F:75:TYR:CD2	1:F:75:TYR:C	2.93	0.41
1:A:217:VAL:HG13	1:A:226:LEU:HD12	2.02	0.41
1:A:118:LYS:HG3	1:A:145:ILE:HG22	2.02	0.41
1:C:194:LYS:HG3	1:C:194:LYS:H	1.67	0.41
1:E:221:ASN:C	1:E:221:ASN:HD22	2.24	0.41
1:D:217:VAL:HG13	1:D:226:LEU:HD23	2.03	0.41
1:B:89:ASP:HB2	4:B:1261:HOH:O	2.19	0.41
1:B:113:ILE:HA	1:B:113:ILE:HD12	1.93	0.41
1:E:77:VAL:HG11	1:F:35:VAL:HG21	2.03	0.41
1:A:92:ARG:O	1:A:97:LYS:HA	2.20	0.41
1:G:91:ILE:HG13	1:G:131:PHE:HZ	1.85	0.41
1:D:37:ARG:NH2	1:D:149:ALA:O	2.53	0.41
1:F:44:VAL:HG13	1:F:45:GLY:N	2.35	0.41
1:C:39:LYS:NZ	1:C:39:LYS:HB2	2.36	0.41
1:D:189:ASP:OD2	1:D:189:ASP:N	2.51	0.41
1:G:31:GLN:HE21	1:H:171:LYS:NZ	2.19	0.41
1:D:54:THR:HA	1:D:127:CYS:O	2.20	0.41
1:C:35:VAL:HG13	1:C:39:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:SER:OG	1:C:130:SER:HB3	2.20	0.41
1:B:166:GLU:HG2	1:B:174:TYR:CG	2.56	0.40
1:C:55:ILE:HD13	1:C:154:PHE:HD1	1.86	0.40
4:A:1217:HOH:O	1:C:175:LYS:HE2	2.21	0.40
1:E:205:ASP:OD2	1:E:205:ASP:N	2.46	0.40
1:H:203:LYS:O	1:H:207:CYS:HB3	2.22	0.40
1:B:118:LYS:O	1:B:118:LYS:HG2	2.21	0.40
1:B:85:THR:HA	1:B:128:ILE:O	2.22	0.40
1:B:163:HIS:HA	4:B:1244:HOH:O	2.22	0.40
1:B:106:ARG:NH2	1:B:186:THR:OG1	2.55	0.40
1:E:106:ARG:HH22	3:E:1500:ADX:C2	2.34	0.40
1:D:96:ASN:OD1	1:D:112:ARG:HD2	2.22	0.40
1:C:132:ILE:O	1:C:133:SER:C	2.59	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1117:HOH:O	4:C:1392:HOH:O[2_556]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	199/208 (96%)	190 (96%)	8 (4%)	1 (0%)	34 22
1	B	191/208 (92%)	185 (97%)	4 (2%)	2 (1%)	19 8
1	C	202/208 (97%)	196 (97%)	5 (2%)	1 (0%)	34 22
1	D	202/208 (97%)	194 (96%)	8 (4%)	0	100 100
1	E	201/208 (97%)	195 (97%)	6 (3%)	0	100 100
1	F	202/208 (97%)	195 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	199/208 (96%)	194 (98%)	4 (2%)	1 (0%)	34 22
1	H	191/208 (92%)	184 (96%)	7 (4%)	0	100 100
All	All	1587/1664 (95%)	1533 (97%)	49 (3%)	5 (0%)	46 36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLY
1	B	48	GLY
1	G	169	ASP
1	B	169	ASP
1	C	169	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	170/175 (97%)	160 (94%)	10 (6%)	24 14
1	B	163/175 (93%)	154 (94%)	9 (6%)	27 16
1	C	171/175 (98%)	162 (95%)	9 (5%)	28 17
1	D	171/175 (98%)	163 (95%)	8 (5%)	32 23
1	E	167/175 (95%)	155 (93%)	12 (7%)	18 9
1	F	169/175 (97%)	162 (96%)	7 (4%)	37 28
1	G	168/175 (96%)	161 (96%)	7 (4%)	36 28
1	H	162/175 (93%)	152 (94%)	10 (6%)	23 13
All	All	1341/1400 (96%)	1269 (95%)	72 (5%)	27 17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	38	ASN

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Mol	Chain	Res	Type
1	A	46	THR
1	A	93	GLN
1	A	176	LYS
1	A	183	LYS
1	A	208	ASP
1	A	218	GLU
1	A	220	LEU
1	A	222	GLU
1	B	46	THR
1	B	72	LEU
1	B	74	GLU
1	B	89	ASP
1	B	93	GLN
1	B	98	ASN
1	B	99	LEU
1	B	137	GLN
1	B	170	VAL
1	C	28	VAL
1	C	39	LYS
1	C	44	VAL
1	C	46	THR
1	C	69	SER
1	C	74	GLU
1	C	137	GLN
1	C	175	LYS
1	C	194	LYS
1	D	26	THR
1	D	44	VAL
1	D	47	ARG
1	D	60	LEU
1	D	81	ILE
1	D	167	GLN
1	D	205	ASP
1	D	224	ASP
1	E	35	VAL
1	E	46	THR
1	E	167	GLN
1	E	190	SER
1	E	191	GLU
1	E	194	LYS
1	E	202	LEU
1	E	205	ASP

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Mol	Chain	Res	Type
1	E	206	SER
1	E	208	ASP
1	E	214	GLN
1	E	221	ASN
1	F	98	ASN
1	F	118	LYS
1	F	130	SER
1	F	137	GLN
1	F	168	ARG
1	F	208	ASP
1	F	226	LEU
1	G	89	ASP
1	G	170	VAL
1	G	183	LYS
1	G	191	GLU
1	G	203	LYS
1	G	207	CYS
1	G	223	ARG
1	H	51	ARG
1	H	55	ILE
1	H	130	SER
1	H	150	SER
1	H	167	GLN
1	H	196	GLU
1	H	203	LYS
1	H	211	ASP
1	H	214	GLN
1	H	222	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	210	ASN
1	A	215	GLN
1	A	221	ASN
1	B	38	ASN
1	B	93	GLN
1	B	98	ASN
1	B	144	GLN
1	B	210	ASN
1	B	214	GLN

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Mol	Chain	Res	Type
1	C	27	ASN
1	C	38	ASN
1	C	93	GLN
1	C	109	ASN
1	C	167	GLN
1	C	210	ASN
1	C	221	ASN
1	D	27	ASN
1	D	38	ASN
1	D	79	HIS
1	D	90	ASN
1	D	221	ASN
1	E	38	ASN
1	E	140	ASN
1	E	167	GLN
1	E	221	ASN
1	F	31	GLN
1	F	98	ASN
1	F	215	GLN
1	G	27	ASN
1	G	31	GLN
1	G	93	GLN
1	G	167	GLN
1	G	214	GLN
1	G	221	ASN
1	H	90	ASN
1	H	93	GLN
1	H	167	GLN
1	H	210	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	ADX	A	1100	-	22,29,29	1.21	2 (9%)	25,45,45	2.09	4 (16%)
3	ADX	A	1101	-	22,29,29	1.10	2 (9%)	25,45,45	1.89	4 (16%)
3	ADX	B	1200	-	22,29,29	1.16	1 (4%)	25,45,45	1.84	4 (16%)
3	ADX	B	1201	2	22,29,29	1.09	2 (9%)	25,45,45	1.99	6 (24%)
3	ADX	C	1300	-	22,29,29	1.02	1 (4%)	25,45,45	1.95	5 (20%)
3	ADX	C	1301	2	22,29,29	1.16	2 (9%)	25,45,45	1.81	2 (8%)
3	ADX	D	1400	-	22,29,29	0.85	1 (4%)	25,45,45	2.37	5 (20%)
3	ADX	D	1401	2	22,29,29	1.12	1 (4%)	25,45,45	1.87	2 (8%)
3	ADX	E	1500	-	22,29,29	1.26	2 (9%)	25,45,45	1.83	2 (8%)
3	ADX	E	1501	2	22,29,29	1.08	1 (4%)	25,45,45	1.86	3 (12%)
3	ADX	F	1600	-	22,29,29	1.20	2 (9%)	25,45,45	1.80	4 (16%)
3	ADX	F	1601	2	22,29,29	1.17	1 (4%)	25,45,45	1.81	3 (12%)
3	ADX	G	1700	-	22,29,29	1.01	2 (9%)	25,45,45	2.20	6 (24%)
3	ADX	G	1701	-	22,29,29	1.06	1 (4%)	25,45,45	1.82	3 (12%)
3	ADX	H	1800	-	22,29,29	1.16	2 (9%)	25,45,45	2.26	5 (20%)
3	ADX	H	1801	2	22,29,29	1.09	2 (9%)	25,45,45	1.89	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADX	A	1100	-	-	0/6/32/32	0/3/3/3
3	ADX	A	1101	-	-	0/6/32/32	0/3/3/3
3	ADX	B	1200	-	-	0/6/32/32	0/3/3/3
3	ADX	B	1201	2	-	0/6/32/32	0/3/3/3
3	ADX	C	1300	-	-	0/6/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADX	C	1301	2	-	0/6/32/32	0/3/3/3
3	ADX	D	1400	-	-	0/6/32/32	0/3/3/3
3	ADX	D	1401	2	-	0/6/32/32	0/3/3/3
3	ADX	E	1500	-	-	0/6/32/32	0/3/3/3
3	ADX	E	1501	2	-	0/6/32/32	0/3/3/3
3	ADX	F	1600	-	-	0/6/32/32	0/3/3/3
3	ADX	F	1601	2	-	0/6/32/32	0/3/3/3
3	ADX	G	1700	-	-	0/6/32/32	0/3/3/3
3	ADX	G	1701	-	-	0/6/32/32	0/3/3/3
3	ADX	H	1800	-	-	0/6/32/32	0/3/3/3
3	ADX	H	1801	2	-	0/6/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1400	ADX	C5-C4	2.11	1.45	1.40
3	A	1101	ADX	O4'-C1'	2.13	1.43	1.41
3	C	1301	ADX	O4'-C1'	2.26	1.44	1.41
3	B	1201	ADX	O4'-C1'	2.29	1.44	1.41
3	H	1801	ADX	O4'-C1'	2.31	1.44	1.41
3	G	1700	ADX	O4'-C1'	2.34	1.44	1.41
3	G	1700	ADX	C5-C4	2.59	1.46	1.40
3	A	1100	ADX	C5-C4	2.80	1.46	1.40
3	H	1800	ADX	O4'-C1'	3.00	1.45	1.41
3	E	1500	ADX	C5-C4	3.08	1.47	1.40
3	F	1600	ADX	C5-C4	3.24	1.47	1.40
3	F	1600	ADX	O4'-C1'	3.26	1.45	1.41
3	H	1801	ADX	C5-C4	3.28	1.47	1.40
3	B	1201	ADX	C5-C4	3.32	1.48	1.40
3	A	1101	ADX	C5-C4	3.32	1.48	1.40
3	E	1501	ADX	C5-C4	3.32	1.48	1.40
3	C	1300	ADX	C5-C4	3.35	1.48	1.40
3	D	1401	ADX	C5-C4	3.35	1.48	1.40
3	G	1701	ADX	C5-C4	3.37	1.48	1.40
3	H	1800	ADX	C5-C4	3.40	1.48	1.40
3	C	1301	ADX	C5-C4	3.46	1.48	1.40
3	B	1200	ADX	C5-C4	3.61	1.48	1.40
3	F	1601	ADX	C5-C4	3.62	1.48	1.40
3	A	1100	ADX	O4'-C1'	3.72	1.45	1.41
3	E	1500	ADX	O4'-C1'	3.87	1.46	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1400	ADX	N3-C2-N1	-9.56	121.58	128.89
3	H	1800	ADX	N3-C2-N1	-8.52	122.37	128.89
3	A	1100	ADX	N3-C2-N1	-8.16	122.65	128.89
3	G	1700	ADX	N3-C2-N1	-7.65	123.04	128.89
3	D	1401	ADX	N3-C2-N1	-7.60	123.08	128.89
3	E	1501	ADX	N3-C2-N1	-7.56	123.11	128.89
3	C	1300	ADX	N3-C2-N1	-7.40	123.23	128.89
3	A	1101	ADX	N3-C2-N1	-7.14	123.43	128.89
3	G	1701	ADX	N3-C2-N1	-7.14	123.43	128.89
3	E	1500	ADX	N3-C2-N1	-6.90	123.61	128.89
3	B	1200	ADX	N3-C2-N1	-6.76	123.72	128.89
3	C	1301	ADX	N3-C2-N1	-6.64	123.81	128.89
3	H	1801	ADX	N3-C2-N1	-6.63	123.82	128.89
3	B	1201	ADX	N3-C2-N1	-6.58	123.86	128.89
3	F	1600	ADX	N3-C2-N1	-6.37	124.02	128.89
3	F	1601	ADX	N3-C2-N1	-6.25	124.11	128.89
3	C	1301	ADX	C4-C5-N7	-3.66	106.11	109.48
3	H	1801	ADX	C4-C5-N7	-3.47	106.28	109.48
3	D	1400	ADX	O4'-C1'-N9	-3.25	101.29	108.10
3	G	1700	ADX	C4-C5-N7	-3.12	106.61	109.48
3	G	1701	ADX	C4-C5-N7	-3.09	106.63	109.48
3	B	1201	ADX	C4-C5-N7	-3.04	106.68	109.48
3	B	1200	ADX	C4-C5-N7	-2.95	106.76	109.48
3	F	1601	ADX	C4-C5-N7	-2.92	106.79	109.48
3	B	1201	ADX	O3A-PA-O5'	-2.87	95.39	102.97
3	H	1801	ADX	C2'-C1'-N9	-2.80	110.02	114.29
3	F	1600	ADX	C4-C5-N7	-2.78	106.92	109.48
3	D	1401	ADX	C4-C5-N7	-2.77	106.93	109.48
3	A	1101	ADX	C4-C5-N7	-2.74	106.95	109.48
3	E	1501	ADX	C4-C5-N7	-2.73	106.97	109.48
3	G	1700	ADX	O2'-C2'-C3'	-2.72	102.98	111.83
3	G	1701	ADX	O3A-PA-O5'	-2.71	95.82	102.97
3	H	1800	ADX	C4-C5-N7	-2.69	107.00	109.48
3	G	1700	ADX	O4'-C1'-N9	-2.59	102.67	108.10
3	A	1101	ADX	C2'-C1'-N9	-2.55	110.39	114.29
3	A	1100	ADX	O3A-PA-O5'	-2.50	96.38	102.97
3	E	1500	ADX	C4-C5-N7	-2.39	107.28	109.48
3	B	1201	ADX	C2'-C1'-N9	-2.24	110.86	114.29
3	A	1101	ADX	O3A-PA-O5'	-2.20	97.17	102.97
3	A	1100	ADX	C5'-C4'-C3'	-2.19	106.51	115.21
3	C	1300	ADX	O4'-C1'-N9	-2.11	103.68	108.10
3	D	1400	ADX	C4-C5-N7	-2.03	107.61	109.48
3	A	1100	ADX	C4-C5-N7	-2.03	107.61	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1300	ADX	C4-C5-N7	-2.01	107.63	109.48
3	F	1600	ADX	O3B-SB-O2B	2.07	116.33	108.56
3	D	1400	ADX	C2-N1-C6	2.12	122.56	118.77
3	F	1601	ADX	O2A-PA-O3A	2.18	112.72	104.94
3	B	1200	ADX	O2A-PA-O3A	2.22	112.85	104.94
3	E	1501	ADX	C2-N1-C6	2.22	122.73	118.77
3	F	1600	ADX	C2'-C1'-N9	2.24	117.71	114.29
3	B	1200	ADX	C2-N1-C6	2.38	123.02	118.77
3	H	1801	ADX	O2A-PA-O3A	2.39	113.47	104.94
3	H	1800	ADX	C2-N1-C6	2.41	123.08	118.77
3	H	1801	ADX	O4'-C1'-N9	2.54	113.42	108.10
3	B	1201	ADX	O2A-PA-O3A	2.57	114.10	104.94
3	G	1700	ADX	C4'-O4'-C1'	2.64	112.62	109.72
3	D	1400	ADX	C2'-C1'-N9	2.66	118.36	114.29
3	C	1300	ADX	C4'-O4'-C1'	2.71	112.69	109.72
3	H	1800	ADX	C4'-O4'-C1'	3.02	113.03	109.72
3	H	1800	ADX	C2'-C1'-N9	3.07	118.98	114.29
3	C	1300	ADX	C2'-C1'-N9	3.17	119.13	114.29
3	B	1201	ADX	O4'-C1'-N9	3.54	115.52	108.10
3	G	1700	ADX	C2'-C1'-N9	3.91	120.27	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1201	ADX	2	0
3	C	1300	ADX	1	0
3	C	1301	ADX	2	0
3	D	1401	ADX	3	0
3	E	1500	ADX	1	0
3	F	1601	ADX	2	0
3	G	1700	ADX	1	0
3	G	1701	ADX	2	0

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	200/208 (96%)	0.30	12 (6%)	25	28	13, 26, 44, 47	0
1	B	193/208 (92%)	0.12	10 (5%)	31	36	14, 25, 43, 52	0
1	C	204/208 (98%)	0.03	5 (2%)	61	67	13, 24, 40, 45	0
1	D	204/208 (98%)	0.21	10 (4%)	33	38	13, 26, 44, 54	0
1	E	203/208 (97%)	0.08	8 (3%)	43	48	15, 28, 42, 50	0
1	F	204/208 (98%)	0.09	10 (4%)	33	38	15, 26, 45, 49	1 (0%)
1	G	201/208 (96%)	0.37	12 (5%)	25	28	14, 29, 45, 47	0
1	H	193/208 (92%)	0.19	5 (2%)	59	65	15, 27, 43, 47	0
All	All	1602/1664 (96%)	0.17	72 (4%)	37	42	13, 26, 44, 54	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	TYR	6.2
1	F	30	TYR	5.4
1	H	46	THR	5.4
1	G	30	TYR	5.2
1	G	46	THR	5.2
1	A	45	GLY	4.2
1	B	227	PRO	4.1
1	B	47	ARG	4.0
1	G	48	GLY	4.1
1	E	46	THR	4.0
1	D	46	THR	4.0
1	D	163	HIS	3.9
1	D	30	TYR	3.8
1	B	46	THR	3.8
1	D	170	VAL	3.8
1	C	47	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	227	PRO	3.4
1	D	48	GLY	3.3
1	D	167	GLN	3.2
1	A	47	ARG	3.2
1	G	170	VAL	3.1
1	F	26	THR	3.0
1	A	89[A]	ASP	3.0
1	A	222	GLU	2.9
1	E	49	GLY	2.9
1	B	48	GLY	2.8
1	D	25	ALA	2.8
1	A	208	ASP	2.8
1	G	197	ALA	2.8
1	F	46	THR	2.8
1	A	220	LEU	2.8
1	H	211	ASP	2.7
1	E	47	ARG	2.7
1	C	46	THR	2.6
1	G	98	ASN	2.6
1	D	26	THR	2.6
1	A	46	THR	2.5
1	A	32	ALA	2.5
1	B	224	ASP	2.5
1	G	179	ALA	2.5
1	H	98	ASN	2.5
1	G	176	LYS	2.5
1	B	42	GLN	2.5
1	F	25	ALA	2.4
1	C	224	ASP	2.4
1	C	38	ASN	2.4
1	F	24	ARG	2.3
1	G	42	GLN	2.3
1	H	224	ASP	2.3
1	F	197	ALA	2.3
1	E	48	GLY	2.3
1	C	212	CYS	2.2
1	A	224	ASP	2.2
1	E	142	ALA	2.2
1	A	78	CYS	2.2
1	B	225	ILE	2.2
1	F	32	ALA	2.2
1	F	167	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	208	ASP	2.2
1	B	226	LEU	2.2
1	B	209	VAL	2.2
1	E	218	GLU	2.2
1	G	44	VAL	2.1
1	B	45	GLY	2.1
1	D	45	GLY	2.1
1	F	49	GLY	2.1
1	G	180	GLY	2.1
1	D	47	ARG	2.1
1	F	34	HIS	2.1
1	A	167	GLN	2.0
1	G	188	ILE	2.0
1	E	224	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ADX	F	1601	27/27	0.95	0.13	-0.10	19,36,39,39	0
3	ADX	A	1101	27/27	0.94	0.13	-0.23	24,43,44,45	0
3	ADX	E	1500	27/27	0.98	0.10	-0.42	14,16,19,22	0
3	ADX	D	1401	27/27	0.95	0.12	-0.49	21,38,39,40	0
3	ADX	D	1400	27/27	0.98	0.10	-0.52	12,17,20,24	0
3	ADX	H	1801	27/27	0.95	0.12	-0.54	21,33,36,36	0
3	ADX	B	1201	27/27	0.97	0.10	-0.63	21,27,29,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ADX	B	1200	27/27	0.98	0.10	-0.69	12,19,23,26	0
3	ADX	H	1800	27/27	0.97	0.10	-0.70	18,19,23,25	0
3	ADX	F	1600	27/27	0.98	0.09	-0.76	12,18,19,22	0
3	ADX	A	1100	27/27	0.98	0.09	-0.80	13,22,26,27	0
3	ADX	C	1301	27/27	0.94	0.12	-0.82	13,29,30,31	0
3	ADX	C	1300	27/27	0.98	0.09	-0.84	12,17,23,26	0
2	MG	C	1003	1/1	0.99	0.09	-0.88	18,18,18,18	0
3	ADX	G	1701	27/27	0.95	0.11	-0.90	20,40,42,43	0
3	ADX	G	1700	27/27	0.98	0.09	-1.11	15,22,26,28	0
3	ADX	E	1501	27/27	0.97	0.09	-1.13	20,35,37,38	0
2	MG	B	1002	1/1	0.99	0.05	-	18,18,18,18	0
2	MG	H	1008	1/1	0.97	0.11	-	20,20,20,20	0
2	MG	D	1004	1/1	0.99	0.04	-	15,15,15,15	0
2	MG	F	1006	1/1	1.00	0.05	-	19,19,19,19	0
2	MG	E	1005	1/1	0.96	0.18	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.