Full wwPDB X-ray Structure Validation Report (i)

May 23, 2016 – 01:59 PM EDT

PDB ID	:	5CCV
Title	:	Crystal structure of full-length NS5 from dengue virus type 3
Authors	:	Klema, V.J.; Choi, K.H.
Deposited on	:	2015-07-02
Resolution	:	3.60 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:

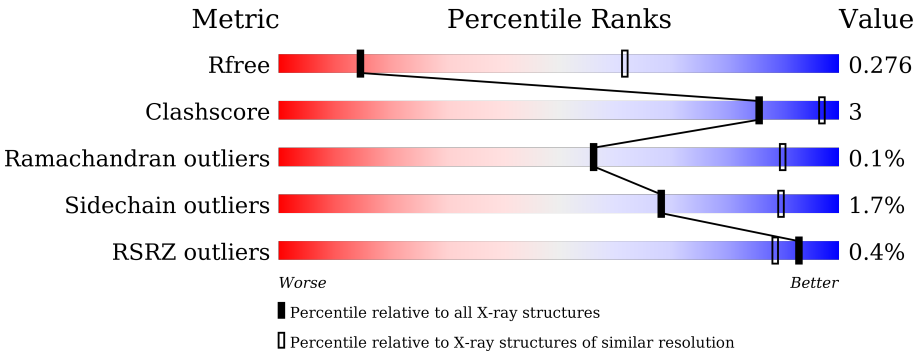
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	905	87% 7% 6%
1	B	905	86% 8% 6%
1	C	905	85% 9% 6%
1	D	905	85% 8% • 6%
1	E	905	% 84% 9% • 6%
1	F	905	86% 7% • 6%

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Mol	Chain	Length	Quality of chain
1	G	905	86% 8% 6%
1	H	905	% 80% 15%

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
3	SAH	H	1003	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 52681 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 RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6831	4301	1229	1255	46			
1	B	851	Total	C	N	O	S	0	0	0
			6892	4346	1236	1263	47			
1	C	852	Total	C	N	O	S	0	0	0
			6879	4339	1229	1263	48			
1	D	848	Total	C	N	O	S	0	0	0
			6827	4302	1226	1252	47			
1	E	852	Total	C	N	O	S	0	0	0
			6885	4341	1231	1266	47			
1	F	850	Total	C	N	O	S	0	0	0
			6846	4311	1231	1257	47			
1	G	847	Total	C	N	O	S	0	0	0
			6813	4292	1222	1252	47			
1	H	767	Total	C	N	O	S	0	0	0
			4484	2739	870	866	9			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	ALA	THR	conflict	UNP P27915
A	?	-	TRP	deletion	UNP P27915
A	?	-	SER	deletion	UNP P27915
A	?	-	ILE	deletion	UNP P27915
A	?	-	HIS	deletion	UNP P27915
A	?	-	ALA	deletion	UNP P27915
A	?	-	HIS	deletion	UNP P27915
A	901	ALA	-	expression tag	UNP P27915
A	902	ALA	-	expression tag	UNP P27915
A	903	ALA	-	expression tag	UNP P27915
A	904	LEU	-	expression tag	UNP P27915
A	905	GLU	-	expression tag	UNP P27915
A	906	HIS	-	expression tag	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
A	907	HIS	-	expression tag	UNP P27915
A	908	HIS	-	expression tag	UNP P27915
A	909	HIS	-	expression tag	UNP P27915
A	910	HIS	-	expression tag	UNP P27915
A	911	HIS	-	expression tag	UNP P27915
B	763	ALA	THR	conflict	UNP P27915
B	?	-	TRP	deletion	UNP P27915
B	?	-	SER	deletion	UNP P27915
B	?	-	ILE	deletion	UNP P27915
B	?	-	HIS	deletion	UNP P27915
B	?	-	ALA	deletion	UNP P27915
B	?	-	HIS	deletion	UNP P27915
B	901	ALA	-	expression tag	UNP P27915
B	902	ALA	-	expression tag	UNP P27915
B	903	ALA	-	expression tag	UNP P27915
B	904	LEU	-	expression tag	UNP P27915
B	905	GLU	-	expression tag	UNP P27915
B	906	HIS	-	expression tag	UNP P27915
B	907	HIS	-	expression tag	UNP P27915
B	908	HIS	-	expression tag	UNP P27915
B	909	HIS	-	expression tag	UNP P27915
B	910	HIS	-	expression tag	UNP P27915
B	911	HIS	-	expression tag	UNP P27915
C	763	ALA	THR	conflict	UNP P27915
C	?	-	TRP	deletion	UNP P27915
C	?	-	SER	deletion	UNP P27915
C	?	-	ILE	deletion	UNP P27915
C	?	-	HIS	deletion	UNP P27915
C	?	-	ALA	deletion	UNP P27915
C	?	-	HIS	deletion	UNP P27915
C	901	ALA	-	expression tag	UNP P27915
C	902	ALA	-	expression tag	UNP P27915
C	903	ALA	-	expression tag	UNP P27915
C	904	LEU	-	expression tag	UNP P27915
C	905	GLU	-	expression tag	UNP P27915
C	906	HIS	-	expression tag	UNP P27915
C	907	HIS	-	expression tag	UNP P27915
C	908	HIS	-	expression tag	UNP P27915
C	909	HIS	-	expression tag	UNP P27915
C	910	HIS	-	expression tag	UNP P27915
C	911	HIS	-	expression tag	UNP P27915
D	763	ALA	THR	conflict	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	TRP	deletion	UNP P27915
D	?	-	SER	deletion	UNP P27915
D	?	-	ILE	deletion	UNP P27915
D	?	-	HIS	deletion	UNP P27915
D	?	-	ALA	deletion	UNP P27915
D	?	-	HIS	deletion	UNP P27915
D	901	ALA	-	expression tag	UNP P27915
D	902	ALA	-	expression tag	UNP P27915
D	903	ALA	-	expression tag	UNP P27915
D	904	LEU	-	expression tag	UNP P27915
D	905	GLU	-	expression tag	UNP P27915
D	906	HIS	-	expression tag	UNP P27915
D	907	HIS	-	expression tag	UNP P27915
D	908	HIS	-	expression tag	UNP P27915
D	909	HIS	-	expression tag	UNP P27915
D	910	HIS	-	expression tag	UNP P27915
D	911	HIS	-	expression tag	UNP P27915
E	763	ALA	THR	conflict	UNP P27915
E	?	-	TRP	deletion	UNP P27915
E	?	-	SER	deletion	UNP P27915
E	?	-	ILE	deletion	UNP P27915
E	?	-	HIS	deletion	UNP P27915
E	?	-	ALA	deletion	UNP P27915
E	?	-	HIS	deletion	UNP P27915
E	901	ALA	-	expression tag	UNP P27915
E	902	ALA	-	expression tag	UNP P27915
E	903	ALA	-	expression tag	UNP P27915
E	904	LEU	-	expression tag	UNP P27915
E	905	GLU	-	expression tag	UNP P27915
E	906	HIS	-	expression tag	UNP P27915
E	907	HIS	-	expression tag	UNP P27915
E	908	HIS	-	expression tag	UNP P27915
E	909	HIS	-	expression tag	UNP P27915
E	910	HIS	-	expression tag	UNP P27915
E	911	HIS	-	expression tag	UNP P27915
F	763	ALA	THR	conflict	UNP P27915
F	?	-	TRP	deletion	UNP P27915
F	?	-	SER	deletion	UNP P27915
F	?	-	ILE	deletion	UNP P27915
F	?	-	HIS	deletion	UNP P27915
F	?	-	ALA	deletion	UNP P27915
F	?	-	HIS	deletion	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
F	901	ALA	-	expression tag	UNP P27915
F	902	ALA	-	expression tag	UNP P27915
F	903	ALA	-	expression tag	UNP P27915
F	904	LEU	-	expression tag	UNP P27915
F	905	GLU	-	expression tag	UNP P27915
F	906	HIS	-	expression tag	UNP P27915
F	907	HIS	-	expression tag	UNP P27915
F	908	HIS	-	expression tag	UNP P27915
F	909	HIS	-	expression tag	UNP P27915
F	910	HIS	-	expression tag	UNP P27915
F	911	HIS	-	expression tag	UNP P27915
G	763	ALA	THR	conflict	UNP P27915
G	?	-	TRP	deletion	UNP P27915
G	?	-	SER	deletion	UNP P27915
G	?	-	ILE	deletion	UNP P27915
G	?	-	HIS	deletion	UNP P27915
G	?	-	ALA	deletion	UNP P27915
G	?	-	HIS	deletion	UNP P27915
G	901	ALA	-	expression tag	UNP P27915
G	902	ALA	-	expression tag	UNP P27915
G	903	ALA	-	expression tag	UNP P27915
G	904	LEU	-	expression tag	UNP P27915
G	905	GLU	-	expression tag	UNP P27915
G	906	HIS	-	expression tag	UNP P27915
G	907	HIS	-	expression tag	UNP P27915
G	908	HIS	-	expression tag	UNP P27915
G	909	HIS	-	expression tag	UNP P27915
G	910	HIS	-	expression tag	UNP P27915
G	911	HIS	-	expression tag	UNP P27915
H	763	ALA	THR	conflict	UNP P27915
H	?	-	TRP	deletion	UNP P27915
H	?	-	SER	deletion	UNP P27915
H	?	-	ILE	deletion	UNP P27915
H	?	-	HIS	deletion	UNP P27915
H	?	-	ALA	deletion	UNP P27915
H	?	-	HIS	deletion	UNP P27915
H	901	ALA	-	expression tag	UNP P27915
H	902	ALA	-	expression tag	UNP P27915
H	903	ALA	-	expression tag	UNP P27915
H	904	LEU	-	expression tag	UNP P27915
H	905	GLU	-	expression tag	UNP P27915
H	906	HIS	-	expression tag	UNP P27915

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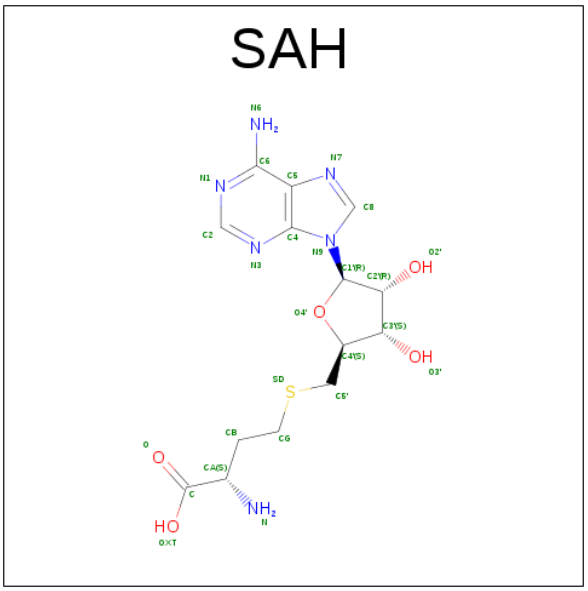
Chain	Residue	Modelled	Actual	Comment	Reference
H	907	HIS	-	expression tag	UNP P27915
H	908	HIS	-	expression tag	UNP P27915
H	909	HIS	-	expression tag	UNP P27915
H	910	HIS	-	expression tag	UNP P27915
H	911	HIS	-	expression tag	UNP P27915

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



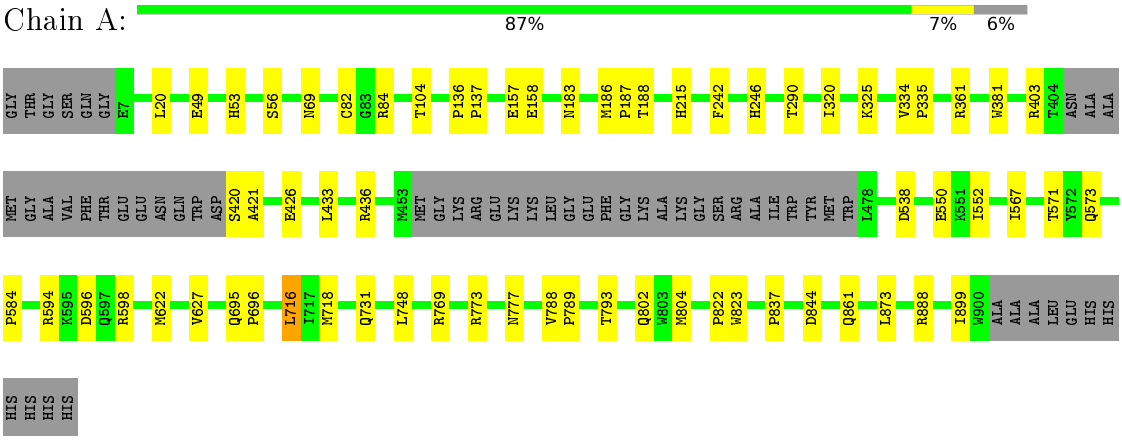
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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.

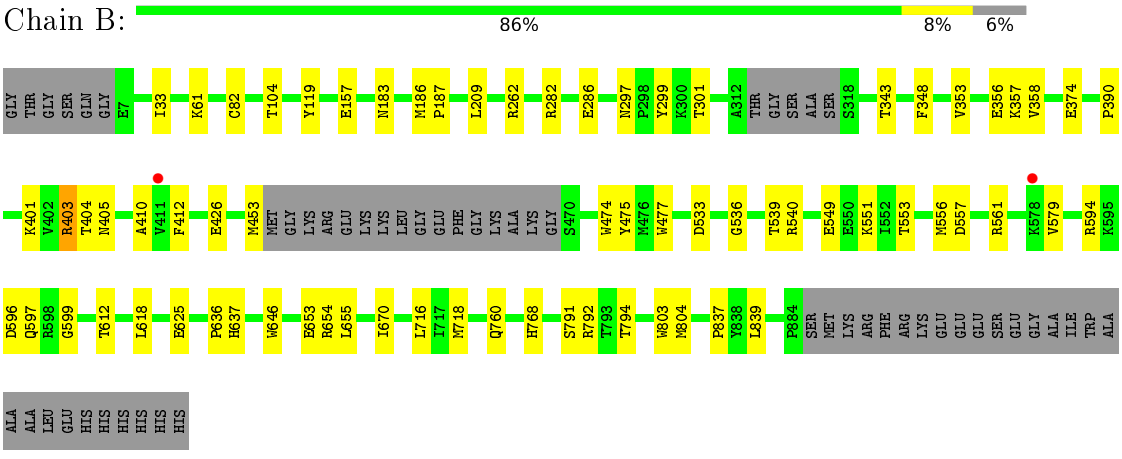
- Molecule 1: RNA-directed RNA polymerase NS5

Chain A:



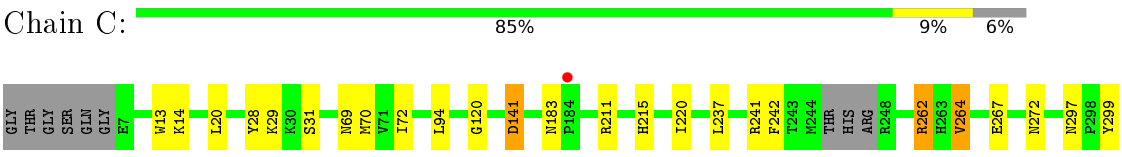
- Molecule 1: RNA-directed RNA polymerase NS5

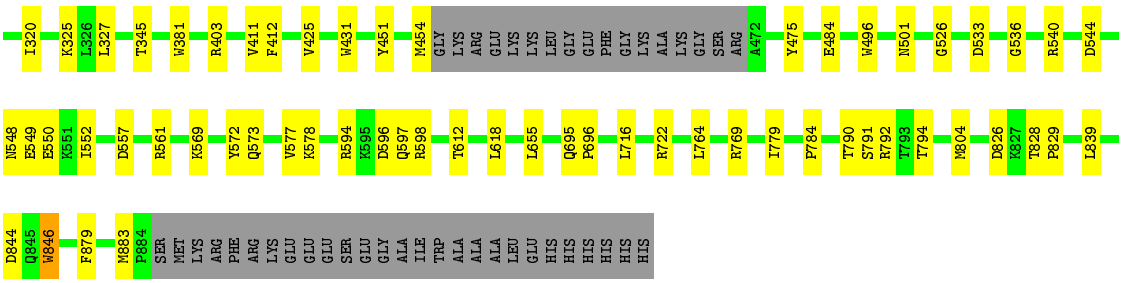
Chain B:



- Molecule 1: RNA-directed RNA polymerase NS5

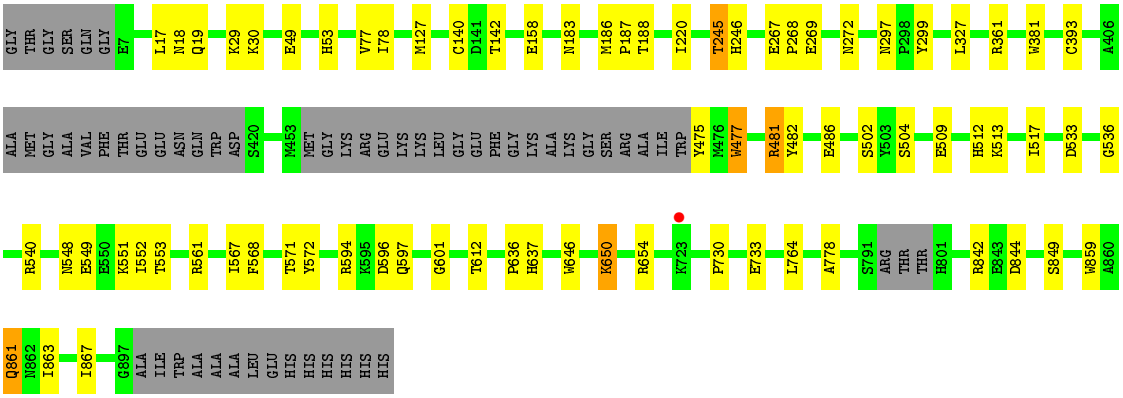
Chain C:





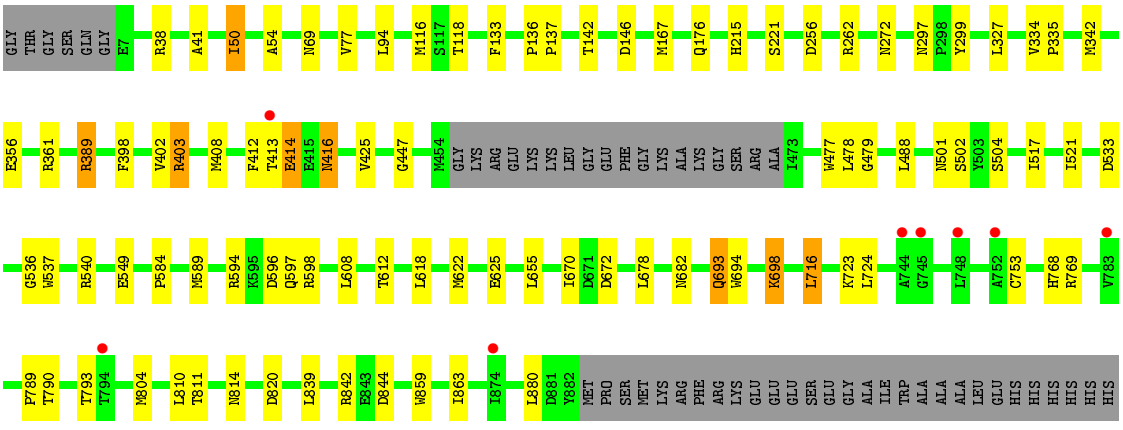
• Molecule 1: RNA-directed RNA polymerase NS5

Chain D:



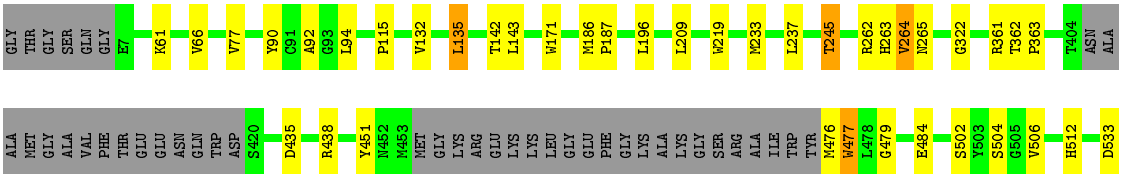
• Molecule 1: RNA-directed RNA polymerase NS5

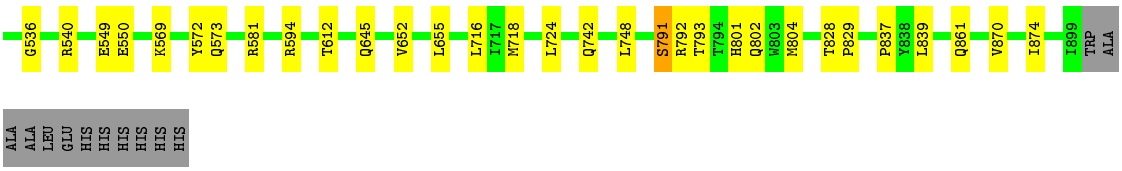
Chain E:



• Molecule 1: RNA-directed RNA polymerase NS5

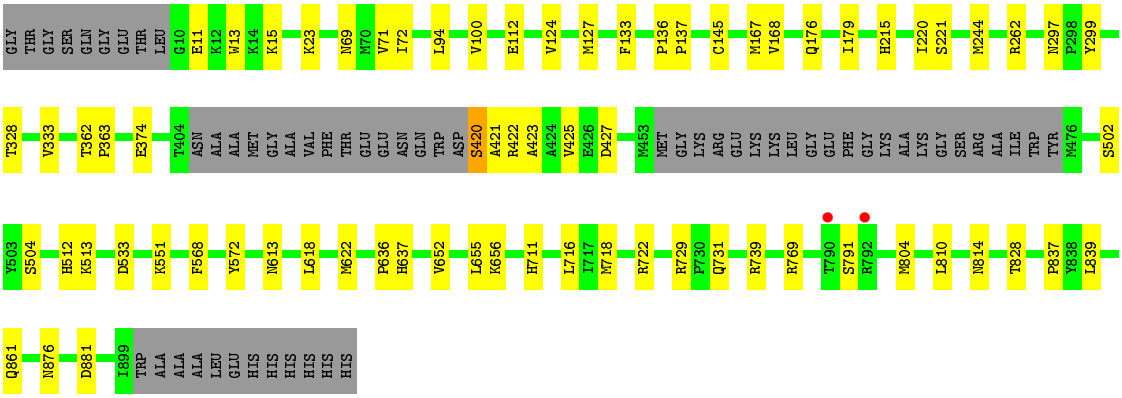
Chain F:





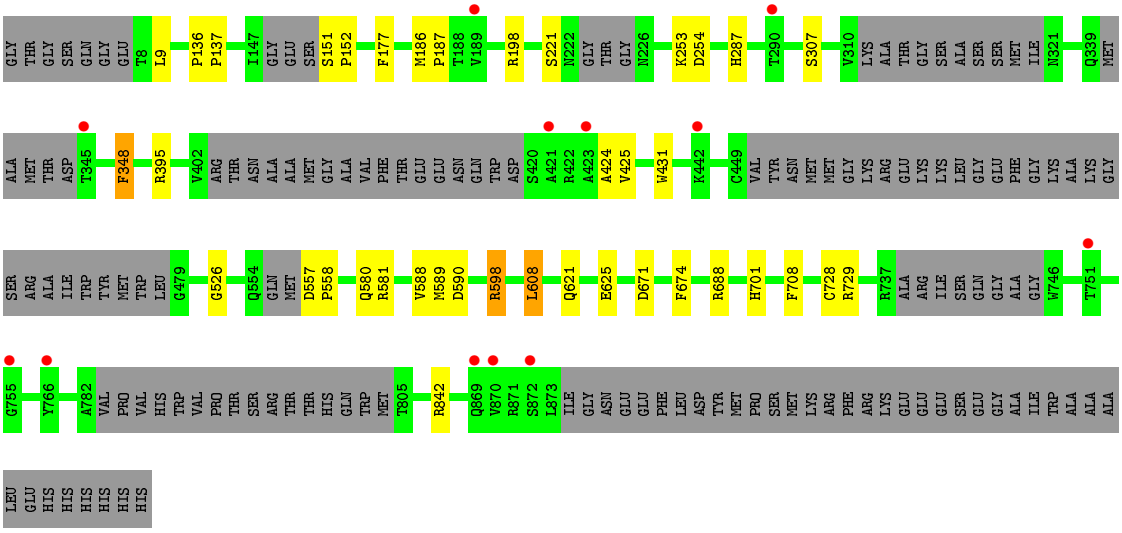
• Molecule 1: RNA-directed RNA polymerase NS5

Chain G:



• Molecule 1: RNA-directed RNA polymerase NS5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.31Å 215.31Å 480.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 3.60 49.22 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-3.60) 94.3 (49.22-3.60)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.238 , 0.274 0.243 , 0.276	Depositor DCC
R_{free} test set	1876 reflections (1.33%)	DCC
Wilson B-factor (Å^2)	86.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	52681	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: ZN, SAH

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	0.20	0/6992	0.36	1/9454 (0.0%)
1	B	0.21	0/7060	0.36	0/9551
1	C	0.21	0/7046	0.36	0/9533
1	D	0.21	0/6990	0.36	0/9452
1	E	0.21	0/7053	0.36	0/9544
1	F	0.21	0/7009	0.36	0/9477
1	G	0.21	0/6976	0.36	0/9434
1	H	0.19	0/4563	0.35	0/6318
All	All	0.21	0/53689	0.36	1/72763 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	716	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6831	0	6746	35	0
1	B	6892	0	6803	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6879	0	6788	43	0
1	D	6827	0	6724	48	0
1	E	6885	0	6788	51	0
1	F	6846	0	6757	36	0
1	G	6813	0	6712	40	0
1	H	4484	0	2810	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	F	26	0	19	0	0
3	G	26	0	19	0	0
3	H	26	0	19	0	0
All	All	52681	0	50280	290	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 3.

All (290) 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:G:420:SER:O	1:G:422:ARG:N	1.97	0.97
1:A:82:CYS:HG	1:A:104:THR:HG1	1.35	0.72
1:D:361:ARG:HA	1:D:594:ARG:HH22	1.58	0.68
1:D:245:THR:O	1:G:861:GLN:NE2	2.27	0.68
1:G:13:TRP:HZ2	1:G:215:HIS:HB2	1.58	0.67
1:A:899:ILE:HG13	1:F:237:LEU:HD12	1.78	0.66
1:D:475:TYR:C	1:D:477:TRP:H	2.00	0.64
1:G:422:ARG:O	1:G:425:VAL:N	2.30	0.64
1:B:716:LEU:HD21	1:B:839:LEU:HD23	1.80	0.63
1:C:544:ASP:O	1:C:548:ASN:ND2	2.31	0.63
1:B:358:VAL:HG13	1:B:597:GLN:HE22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:CYS:SG	1:B:104:THR:OG1	2.57	0.63
1:G:716:LEU:HD21	1:G:839:LEU:HD23	1.82	0.61
1:G:145:CYS:HB3	1:G:179:ILE:HG23	1.85	0.58
1:D:49:GLU:OE1	1:D:53:HIS:NE2	2.33	0.57
1:B:549:GLU:OE2	1:B:612:THR:OG1	2.22	0.57
1:E:769:ARG:NH1	1:E:844:ASP:OD1	2.38	0.57
1:D:844:ASP:OD1	1:D:849:SER:OG	2.24	0.56
1:G:127:MET:HG2	1:H:526:GLY:HA2	1.88	0.55
1:H:424:ALA:O	1:H:431:TRP:NE1	2.39	0.55
1:A:718:MET:HG2	1:A:837:PRO:HG3	1.89	0.54
1:C:550:GLU:OE1	1:C:573:GLN:NE2	2.41	0.54
1:B:453:MET:HG3	1:B:579:VAL:HB	1.89	0.54
1:H:580:GLN:HA	1:H:589:MET:HA	1.89	0.54
1:D:861:GLN:HG2	1:G:244:MET:HG3	1.90	0.54
1:A:594:ARG:NE	1:A:596:ASP:OD1	2.33	0.53
1:E:327:LEU:O	1:E:859:TRP:NE1	2.39	0.53
1:E:678:LEU:O	1:E:682:ASN:ND2	2.39	0.53
1:F:92:ALA:O	1:F:262:ARG:NH1	2.41	0.53
1:A:567:ILE:O	1:A:571:THR:OG1	2.21	0.52
1:C:425:VAL:HG13	1:C:431:TRP:HZ2	1.74	0.52
1:G:176:GLN:OE1	1:G:221:SER:OG	2.25	0.52
1:B:539:THR:HA	1:B:597:GLN:HG3	1.91	0.52
1:A:769:ARG:NH2	1:A:844:ASP:OD1	2.43	0.52
1:A:49:GLU:OE1	1:A:53:HIS:NE2	2.34	0.51
1:D:482:TYR:O	1:D:486:GLU:N	2.41	0.51
1:A:157:GLU:HB2	1:A:183:ASN:HD22	1.76	0.51
1:B:594:ARG:NE	1:B:596:ASP:OD1	2.44	0.51
1:D:158:GLU:OE2	1:D:188:THR:OG1	2.24	0.51
1:F:94:LEU:O	1:F:262:ARG:NH2	2.44	0.50
1:G:328:THR:OG1	1:G:739:ARG:NH2	2.43	0.50
1:D:327:LEU:O	1:D:859:TRP:NE1	2.43	0.50
1:B:718:MET:HG2	1:B:837:PRO:HG3	1.94	0.50
1:E:537:TRP:HZ2	1:E:612:THR:HG23	1.75	0.50
1:C:716:LEU:HD21	1:C:839:LEU:HD23	1.93	0.49
1:F:484:GLU:OE1	1:F:572:TYR:OH	2.24	0.49
1:E:810:LEU:O	1:E:814:ASN:ND2	2.45	0.49
1:F:791:SER:O	1:F:792:ARG:NE	2.33	0.49
1:G:133:PHE:HD1	1:G:167:MET:HG3	1.78	0.49
1:G:568:PHE:HA	1:G:572:TYR:HB2	1.94	0.49
1:B:401:LYS:O	1:B:403:ARG:NE	2.44	0.49
1:C:791:SER:OG	1:C:792:ARG:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:LEU:O	1:G:262:ARG:NH2	2.46	0.49
1:A:773:ARG:O	1:A:777:ASN:ND2	2.42	0.48
1:A:861:GLN:NE2	1:F:245:THR:O	2.47	0.48
1:D:549:GLU:OE2	1:D:612:THR:OG1	2.31	0.48
1:G:652:VAL:HA	1:G:655:LEU:HD12	1.95	0.48
1:D:475:TYR:C	1:D:477:TRP:N	2.65	0.48
1:C:425:VAL:O	1:C:431:TRP:NE1	2.37	0.48
1:C:496:TRP:O	1:C:501:ASN:ND2	2.46	0.48
1:D:594:ARG:NE	1:D:596:ASP:OD1	2.46	0.48
1:B:82:CYS:HG	1:B:104:THR:HG1	1.41	0.48
1:C:297:ASN:HB2	1:C:299:TYR:HD2	1.79	0.48
1:C:484:GLU:OE1	1:C:572:TYR:OH	2.26	0.48
1:B:374:GLU:HG2	1:B:551:LYS:HE2	1.96	0.48
1:E:693:GLN:HB3	1:E:694:TRP:HD1	1.78	0.48
1:F:263:HIS:O	1:F:265:ASN:N	2.45	0.48
1:A:420:SER:OG	1:A:421:ALA:N	2.45	0.48
1:A:69:ASN:HD22	1:A:584:PRO:HD3	1.79	0.48
1:B:301:THR:HB	1:B:594:ARG:HH12	1.79	0.48
1:H:581:ARG:N	1:H:588:VAL:O	2.43	0.48
1:C:94:LEU:O	1:C:262:ARG:NH2	2.48	0.47
1:D:78:ILE:HD13	1:D:140:CYS:HB3	1.96	0.47
1:B:653:GLU:OE2	1:B:654:ARG:NH1	2.46	0.47
1:H:621:GLN:O	1:H:625:GLU:N	2.45	0.47
1:E:389:ARG:HG2	1:H:842:ARG:HH12	1.79	0.47
1:A:215:HIS:ND1	1:A:215:HIS:O	2.47	0.47
1:C:320:ILE:HG21	1:C:325:LYS:HD2	1.95	0.47
1:E:361:ARG:HA	1:E:594:ARG:HH22	1.78	0.47
1:E:753:CYS:HB2	1:E:789:PRO:HA	1.96	0.47
1:E:215:HIS:ND1	1:E:215:HIS:O	2.46	0.47
1:E:753:CYS:SG	1:E:790:THR:HG22	2.55	0.47
1:G:168:VAL:HG21	1:G:179:ILE:HD13	1.97	0.47
1:B:410:ALA:HB2	1:B:477:TRP:HB3	1.97	0.46
1:E:69:ASN:HD22	1:E:584:PRO:HD3	1.80	0.46
1:G:722:ARG:NH1	1:G:828:THR:O	2.41	0.46
1:C:794:THR:HA	1:C:804:MET:HG3	1.98	0.46
1:F:502:SER:O	1:F:504:SER:N	2.44	0.46
1:F:550:GLU:OE2	1:F:569:LYS:NZ	2.46	0.46
1:A:361:ARG:HA	1:A:594:ARG:HH22	1.80	0.46
1:G:718:MET:HG2	1:G:837:PRO:HG3	1.97	0.46
1:A:433:LEU:HD23	1:A:436:ARG:HH21	1.79	0.46
1:C:549:GLU:OE2	1:C:612:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:550:GLU:OE1	1:F:573:GLN:NE2	2.49	0.46
1:B:536:GLY:O	1:B:540:ARG:HG2	2.16	0.46
1:B:557:ASP:O	1:B:561:ARG:N	2.44	0.45
1:C:549:GLU:OE2	1:C:598:ARG:NH2	2.42	0.45
1:D:475:TYR:HE1	1:D:477:TRP:HD1	1.65	0.45
1:F:132:VAL:HA	1:F:135:LEU:HD23	1.98	0.45
1:G:502:SER:O	1:G:504:SER:N	2.44	0.45
1:B:618:LEU:HD11	1:B:655:LEU:HD21	1.97	0.45
1:C:70:MET:HB3	1:C:220:ILE:HG21	1.97	0.45
1:D:778:ALA:HB1	1:D:867:ILE:HD11	1.97	0.45
1:G:69:ASN:HD22	1:G:72:ILE:HD11	1.80	0.45
1:D:548:ASN:HA	1:D:551:LYS:HE2	1.99	0.45
1:D:650:LYS:HD3	1:D:654:ARG:HH22	1.81	0.45
1:F:536:GLY:O	1:F:540:ARG:HG2	2.17	0.45
1:C:220:ILE:H	1:C:220:ILE:HG13	1.63	0.45
1:D:77:VAL:HG22	1:D:142:THR:HB	1.98	0.45
1:E:536:GLY:O	1:E:540:ARG:HG2	2.16	0.45
1:F:435:ASP:OD1	1:F:438:ARG:NH1	2.49	0.45
1:G:420:SER:C	1:G:422:ARG:N	2.68	0.45
1:D:475:TYR:HE1	1:D:477:TRP:CD1	2.35	0.45
1:B:768:HIS:HB2	1:B:839:LEU:HG	1.99	0.45
1:E:608:LEU:O	1:E:612:THR:HG22	2.17	0.45
1:A:873:LEU:HD11	1:F:322:GLY:HA3	1.98	0.45
1:C:769:ARG:NE	1:C:844:ASP:OD1	2.46	0.44
1:D:29:LYS:HG3	1:D:30:LYS:HG3	1.99	0.44
1:D:475:TYR:CD1	1:D:475:TYR:O	2.70	0.44
1:A:381:TRP:CE3	1:A:552:ILE:HD13	2.52	0.44
1:B:297:ASN:HB2	1:B:299:TYR:HD2	1.83	0.44
1:E:133:PHE:HD1	1:E:167:MET:HG3	1.83	0.44
1:E:94:LEU:O	1:E:262:ARG:NH2	2.50	0.44
1:F:652:VAL:HA	1:F:655:LEU:HD12	2.00	0.44
1:F:870:VAL:O	1:F:874:ILE:HG12	2.17	0.44
1:C:536:GLY:O	1:C:540:ARG:HG2	2.18	0.44
1:F:716:LEU:HD21	1:F:839:LEU:HD23	1.98	0.44
1:E:136:PRO:HA	1:E:137:PRO:HD3	1.88	0.44
1:E:412:PHE:O	1:E:414:GLU:N	2.50	0.44
1:E:693:GLN:HB3	1:E:694:TRP:CD1	2.52	0.44
1:A:748:LEU:HD22	1:F:748:LEU:HD22	1.98	0.44
1:G:297:ASN:HB2	1:G:299:TYR:HD2	1.82	0.44
1:C:784:PRO:HG3	1:C:879:PHE:HE1	1.81	0.44
1:E:594:ARG:NE	1:E:596:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:549:GLU:OE2	1:F:612:THR:OG1	2.35	0.44
1:A:82:CYS:SG	1:A:104:THR:OG1	2.58	0.44
1:D:269:GLU:OE1	1:D:361:ARG:NH2	2.40	0.44
1:D:646:TRP:CH2	1:D:654:ARG:HG3	2.52	0.44
1:G:876:ASN:N	1:G:876:ASN:OD1	2.50	0.44
1:C:13:TRP:HD1	1:C:242:PHE:HE2	1.66	0.44
1:C:183:ASN:OD1	1:C:183:ASN:N	2.50	0.44
1:D:536:GLY:O	1:D:540:ARG:HG2	2.18	0.44
1:G:423:ALA:O	1:G:427:ASP:N	2.50	0.44
1:H:253:LYS:HD3	1:H:254:ASP:N	2.32	0.44
1:E:256:ASP:HB3	1:E:356:GLU:HB3	1.99	0.44
1:E:402:VAL:HG21	1:E:425:VAL:HG11	1.99	0.44
1:E:716:LEU:HD21	1:E:839:LEU:HD23	1.99	0.44
1:E:716:LEU:O	1:E:724:LEU:N	2.47	0.44
1:G:810:LEU:O	1:G:814:ASN:ND2	2.48	0.44
1:B:404:THR:HB	1:B:405:ASN:H	1.67	0.43
1:C:618:LEU:HD11	1:C:655:LEU:HD21	2.00	0.43
1:D:17:LEU:O	1:D:19:GLN:N	2.46	0.43
1:D:267:GLU:H	1:D:268:PRO:HD2	1.82	0.43
1:E:416:ASN:O	1:E:416:ASN:ND2	2.44	0.43
1:E:297:ASN:HB2	1:E:299:TYR:HD2	1.84	0.43
1:B:157:GLU:HB2	1:B:183:ASN:HD22	1.83	0.43
1:B:474:TRP:CE3	1:B:599:GLY:HA2	2.54	0.43
1:E:38:ARG:HD3	1:E:41:ALA:HB3	2.00	0.43
1:F:361:ARG:HA	1:F:594:ARG:NH2	2.34	0.43
1:C:141:ASP:N	1:C:141:ASP:OD1	2.51	0.43
1:C:451:TYR:HB2	1:C:577:VAL:HG22	2.01	0.43
1:F:77:VAL:HG22	1:F:142:THR:HB	2.00	0.43
1:B:390:PRO:HB2	1:B:556:MET:HG2	2.00	0.43
1:B:636:PRO:HG2	1:B:637:HIS:CD2	2.53	0.43
1:D:481:ARG:NH2	1:D:601:GLY:O	2.52	0.43
1:E:618:LEU:HD11	1:E:655:LEU:HD21	1.99	0.43
1:A:136:PRO:HA	1:A:137:PRO:HD3	1.88	0.43
1:C:120:GLY:HA2	1:C:262:ARG:HB2	2.01	0.43
1:D:596:ASP:OD1	1:D:597:GLN:N	2.52	0.43
1:H:425:VAL:HA	1:H:431:TRP:CZ2	2.53	0.43
1:B:282:ARG:O	1:B:286:GLU:HG2	2.19	0.43
1:B:625:GLU:OE1	1:B:646:TRP:NE1	2.37	0.43
1:C:557:ASP:O	1:C:561:ARG:N	2.42	0.43
1:D:512:HIS:CD2	1:D:513:LYS:HG3	2.54	0.43
1:E:768:HIS:H	1:E:768:HIS:CD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:GLN:NE2	1:B:803:TRP:O	2.52	0.43
1:C:596:ASP:OD1	1:C:597:GLN:N	2.52	0.43
1:F:828:THR:HA	1:F:829:PRO:HD3	1.89	0.43
1:G:136:PRO:HA	1:G:137:PRO:HD3	1.89	0.43
1:D:863:ILE:O	1:D:867:ILE:HG12	2.18	0.42
1:E:116:MET:HB3	1:E:118:THR:HG23	2.01	0.42
1:G:636:PRO:HG2	1:G:637:HIS:CD2	2.54	0.42
1:C:381:TRP:CE3	1:C:552:ILE:HD13	2.54	0.42
1:D:220:ILE:HG13	1:D:220:ILE:H	1.63	0.42
1:E:693:GLN:C	1:E:694:TRP:HD1	2.22	0.42
1:F:512:HIS:CD2	1:F:802:GLN:HE22	2.36	0.42
1:G:220:ILE:HG13	1:G:220:ILE:H	1.67	0.42
1:H:136:PRO:HA	1:H:137:PRO:HD3	1.89	0.42
1:A:550:GLU:OE2	1:A:573:GLN:NE2	2.51	0.42
1:D:636:PRO:HG2	1:D:637:HIS:CD2	2.53	0.42
1:E:77:VAL:HG22	1:E:142:THR:HB	2.01	0.42
1:E:334:VAL:HA	1:E:335:PRO:HD3	1.91	0.42
1:H:151:SER:HA	1:H:152:PRO:HD3	1.91	0.42
1:A:822:PRO:HG2	1:A:823:TRP:CE3	2.55	0.42
1:E:50:ILE:H	1:E:50:ILE:HD13	1.85	0.42
1:E:517:ILE:O	1:E:521:ILE:HG13	2.19	0.42
1:F:451:TYR:HA	1:F:476:MET:HB3	2.00	0.42
1:G:100:VAL:HB	1:G:124:VAL:HA	2.01	0.42
1:A:695:GLN:HA	1:A:696:PRO:HD3	1.94	0.42
1:C:594:ARG:NE	1:C:596:ASP:OD1	2.52	0.42
1:F:196:LEU:HB3	1:F:219:TRP:CH2	2.54	0.42
1:B:553:THR:HG22	1:B:556:MET:HE1	2.01	0.42
1:D:842:ARG:HE	1:E:880:LEU:HD11	1.85	0.42
1:H:177:PHE:H	1:H:221:SER:HB3	1.83	0.42
1:E:625:GLU:HG2	1:E:670:ILE:HD11	2.02	0.42
1:E:398:PHE:O	1:E:402:VAL:HG23	2.20	0.42
1:A:622:MET:HB3	1:A:627:VAL:HB	2.01	0.42
1:C:262:ARG:NH1	1:C:267:GLU:OE1	2.53	0.42
1:D:17:LEU:HG	1:D:18:ASN:H	1.84	0.42
1:A:20:LEU:HD11	1:A:242:PHE:HE1	1.85	0.42
1:A:731:GLN:HB2	1:A:769:ARG:HH12	1.84	0.42
1:D:183:ASN:OD1	1:D:186:MET:HG2	2.20	0.42
1:D:297:ASN:HB2	1:D:299:TYR:HD2	1.84	0.42
1:D:568:PHE:HA	1:D:572:TYR:HB2	2.02	0.42
1:D:475:TYR:CG	1:D:475:TYR:O	2.72	0.41
1:D:553:THR:HB	1:D:561:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:GLU:CD	1:E:598:ARG:HH22	2.24	0.41
1:G:215:HIS:O	1:G:215:HIS:ND1	2.51	0.41
1:B:353:VAL:O	1:B:357:LYS:HB2	2.19	0.41
1:B:625:GLU:HG2	1:B:670:ILE:HD11	2.03	0.41
1:C:29:LYS:HE2	1:C:211:ARG:HD2	2.02	0.41
1:C:411:VAL:HG21	1:C:578:LYS:HD2	2.01	0.41
1:C:790:THR:OG1	1:C:791:SER:N	2.54	0.41
1:D:246:HIS:HB2	1:G:861:GLN:HE22	1.85	0.41
1:D:393:CYS:HB2	1:D:486:GLU:HA	2.02	0.41
1:E:176:GLN:OE1	1:E:221:SER:OG	2.33	0.41
1:E:403:ARG:HD2	1:E:403:ARG:H	1.85	0.41
1:D:502:SER:O	1:D:504:SER:N	2.42	0.41
1:D:730:PRO:HB2	1:D:733:GLU:HG3	2.02	0.41
1:C:722:ARG:HD3	1:C:826:ASP:HB3	2.02	0.41
1:F:186:MET:HA	1:F:187:PRO:HD3	1.92	0.41
1:F:716:LEU:N	1:F:724:LEU:O	2.44	0.41
1:G:711:HIS:NE2	1:G:729:ARG:HD2	2.35	0.41
1:C:828:THR:HA	1:C:829:PRO:HD3	1.85	0.41
1:C:526:GLY:HA2	1:D:127:MET:HG3	2.02	0.41
1:F:61:LYS:HA	1:F:209:LEU:HD13	2.03	0.41
1:A:56:SER:HB3	1:A:84:ARG:HD3	2.02	0.41
1:B:61:LYS:HA	1:B:209:LEU:HD12	2.02	0.41
1:B:186:MET:HA	1:B:187:PRO:HD3	1.90	0.41
1:C:237:LEU:O	1:C:241:ARG:HG2	2.20	0.41
1:D:186:MET:HA	1:D:187:PRO:HD3	1.91	0.41
1:C:550:GLU:OE2	1:C:569:LYS:HE3	2.21	0.41
1:D:381:TRP:CE3	1:D:552:ILE:HD13	2.56	0.41
1:D:567:ILE:O	1:D:571:THR:OG1	2.24	0.41
1:G:512:HIS:CD2	1:G:513:LYS:HG3	2.56	0.41
1:G:652:VAL:HG12	1:G:656:LYS:HE3	2.02	0.41
1:H:186:MET:HA	1:H:187:PRO:HD3	1.87	0.41
1:A:158:GLU:OE2	1:A:188:THR:OG1	2.28	0.41
1:H:557:ASP:HA	1:H:558:PRO:HD3	1.93	0.41
1:A:334:VAL:HA	1:A:335:PRO:HD3	1.90	0.41
1:E:477:TRP:CZ2	1:E:479:GLY:HA3	2.55	0.41
1:E:38:ARG:HH22	1:E:54:ALA:HB3	1.86	0.41
1:E:698:LYS:HD3	1:E:698:LYS:H	1.85	0.41
1:F:143:LEU:HD22	1:F:171:TRP:HB2	2.03	0.41
1:F:477:TRP:CZ2	1:F:479:GLY:HA3	2.56	0.41
1:G:731:GLN:HB2	1:G:769:ARG:NH1	2.36	0.41
1:A:246:HIS:N	1:F:861:GLN:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HG21	1:A:325:LYS:HD2	2.03	0.40
1:E:820:ASP:OD2	1:G:23:LYS:NZ	2.53	0.40
1:F:793:THR:HB	1:F:801:HIS:CE1	2.56	0.40
1:F:66:VAL:HG21	1:F:90:TYR:HE2	1.86	0.40
1:G:112:GLU:HB3	1:H:701:HIS:CE1	2.56	0.40
1:G:362:THR:HA	1:G:363:PRO:HD3	1.96	0.40
1:H:598:ARG:CZ	1:H:608:LEU:HG	2.52	0.40
1:A:788:VAL:HA	1:A:789:PRO:HD3	1.87	0.40
1:C:215:HIS:ND1	1:C:215:HIS:O	2.53	0.40
1:E:146:ASP:HB3	3:E:1003:SAH:HG1	2.02	0.40
1:G:13:TRP:HE1	1:G:215:HIS:HD2	1.69	0.40
1:H:307:SER:HA	1:H:590:ASP:HA	2.03	0.40
1:H:348:PHE:HA	1:H:348:PHE:HD1	1.68	0.40
1:H:728:CYS:SG	1:H:729:ARG:N	2.94	0.40
1:A:538:ASP:HB3	1:A:598:ARG:HB3	2.03	0.40
1:B:119:TYR:CE2	1:B:262:ARG:HD2	2.57	0.40
1:C:695:GLN:HA	1:C:696:PRO:HD3	1.93	0.40
1:C:846:TRP:CD1	1:E:842:ARG:HD3	2.57	0.40
1:E:672:ASP:HB3	1:F:115:PRO:HB3	2.04	0.40
1:A:403:ARG:NH2	1:A:426:GLU:OE2	2.53	0.40
1:B:791:SER:OG	1:B:792:ARG:N	2.52	0.40
1:C:327:LEU:HD12	1:C:779:ILE:HG12	2.03	0.40
1:E:502:SER:C	1:E:504:SER:H	2.25	0.40
1:E:596:ASP:HB2	1:E:597:GLN:H	1.69	0.40
1:E:618:LEU:O	1:E:622:MET:HG3	2.21	0.40
1:F:718:MET:HG2	1:F:837:PRO:HG3	2.02	0.40
1:G:618:LEU:O	1:G:622:MET:HG3	2.21	0.40
1:A:186:MET:HA	1:A:187:PRO:HD3	1.91	0.40
1:B:596:ASP:OD1	1:B:597:GLN:N	2.54	0.40
1:C:69:ASN:HD22	1:C:72:ILE:HD11	1.86	0.40
1:D:509:GLU:HG2	1:D:517:ILE:HD11	2.03	0.40
1:F:362:THR:HA	1:F:363:PRO:HD3	1.92	0.40
1:G:374:GLU:HG3	1:G:551:LYS:HE3	2.03	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	843/905 (93%)	811 (96%)	32 (4%)	0	100	100
1	B	845/905 (93%)	806 (95%)	38 (4%)	1 (0%)	56	90
1	C	846/905 (94%)	808 (96%)	37 (4%)	1 (0%)	56	90
1	D	840/905 (93%)	808 (96%)	32 (4%)	0	100	100
1	E	848/905 (94%)	812 (96%)	34 (4%)	2 (0%)	52	87
1	F	844/905 (93%)	804 (95%)	38 (4%)	2 (0%)	52	87
1	G	841/905 (93%)	796 (95%)	42 (5%)	3 (0%)	39	80
1	H	747/905 (82%)	706 (94%)	41 (6%)	0	100	100
All	All	6654/7240 (92%)	6351 (95%)	294 (4%)	9 (0%)	56	90

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	VAL
1	F	264	VAL
1	G	421	ALA
1	G	11	GLU
1	E	413	THR
1	F	791	SER
1	G	791	SER
1	B	33	ILE
1	E	447	GLY

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	739/786 (94%)	733 (99%)	6 (1%)	86 95
1	B	747/786 (95%)	737 (99%)	10 (1%)	76 91
1	C	745/786 (95%)	728 (98%)	17 (2%)	58 85
1	D	737/786 (94%)	729 (99%)	8 (1%)	80 92
1	E	746/786 (95%)	725 (97%)	21 (3%)	51 82
1	F	741/786 (94%)	730 (98%)	11 (2%)	72 90
1	G	736/786 (94%)	728 (99%)	8 (1%)	80 92
1	H	193/786 (25%)	182 (94%)	11 (6%)	25 67
All	All	5384/6288 (86%)	5292 (98%)	92 (2%)	68 89

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	THR
1	A	716	LEU
1	A	793	THR
1	A	802	GLN
1	A	804	MET
1	A	888	ARG
1	B	343	THR
1	B	348	PHE
1	B	356	GLU
1	B	403	ARG
1	B	412	PHE
1	B	426	GLU
1	B	475	TYR
1	B	533	ASP
1	B	794	THR
1	B	804	MET
1	C	14	LYS
1	C	20	LEU
1	C	28	TYR
1	C	31	SER
1	C	141	ASP
1	C	262	ARG
1	C	264	VAL
1	C	272	ASN
1	C	345	THR

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Mol	Chain	Res	Type
1	C	403	ARG
1	C	412	PHE
1	C	454	MET
1	C	475	TYR
1	C	533	ASP
1	C	764	LEU
1	C	846	TRP
1	C	883	MET
1	D	245	THR
1	D	272	ASN
1	D	477	TRP
1	D	481	ARG
1	D	533	ASP
1	D	650	LYS
1	D	764	LEU
1	D	861	GLN
1	E	50	ILE
1	E	272	ASN
1	E	342	MET
1	E	389	ARG
1	E	403	ARG
1	E	408	MET
1	E	414	GLU
1	E	416	ASN
1	E	478	LEU
1	E	488	LEU
1	E	501	ASN
1	E	533	ASP
1	E	589	MET
1	E	693	GLN
1	E	698	LYS
1	E	716	LEU
1	E	723	LYS
1	E	793	THR
1	E	804	MET
1	E	811	THR
1	E	863	ILE
1	F	135	LEU
1	F	233	MET
1	F	245	THR
1	F	264	VAL
1	F	477	TRP

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Mol	Chain	Res	Type
1	F	506	VAL
1	F	533	ASP
1	F	581	ARG
1	F	645	GLN
1	F	742	GLN
1	F	804	MET
1	G	15	LYS
1	G	71	VAL
1	G	333	VAL
1	G	420	SER
1	G	533	ASP
1	G	613	ASN
1	G	804	MET
1	G	881	ASP
1	H	9	LEU
1	H	198	ARG
1	H	287	HIS
1	H	348	PHE
1	H	395	ARG
1	H	598	ARG
1	H	608	LEU
1	H	671	ASP
1	H	674	PHE
1	H	688	ARG
1	H	708	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	562	GLN
1	A	861	GLN
1	B	597	GLN
1	B	704	GLN
1	D	861	GLN
1	F	512	HIS
1	F	742	GLN
1	G	554	GLN
1	G	613	ASN
1	G	617	GLN
1	G	861	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

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	SAH	A	1003	-	22,28,28	1.12	2 (9%)	18,40,40	1.10	0
3	SAH	B	1003	-	22,28,28	1.11	2 (9%)	18,40,40	1.12	0
3	SAH	C	1003	-	22,28,28	1.18	2 (9%)	18,40,40	1.09	0
3	SAH	D	1003	-	22,28,28	1.05	0	18,40,40	1.10	0
3	SAH	E	1003	-	22,28,28	1.07	2 (9%)	18,40,40	1.11	1 (5%)
3	SAH	F	1003	-	22,28,28	1.08	2 (9%)	18,40,40	1.09	1 (5%)
3	SAH	G	1003	-	22,28,28	1.09	2 (9%)	18,40,40	1.08	0
3	SAH	H	1003	-	22,28,28	1.10	2 (9%)	18,40,40	1.10	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	SAH	A	1003	-	-	0/7/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	B	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	C	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	D	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	E	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	F	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	G	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	H	1003	-	-	0/7/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1003	SAH	C2'-C1'	2.01	1.56	1.53
3	E	1003	SAH	C2'-C1'	2.02	1.56	1.53
3	F	1003	SAH	C2'-C1'	2.05	1.56	1.53
3	A	1003	SAH	C2-N3	2.05	1.35	1.32
3	G	1003	SAH	C2-N3	2.05	1.35	1.32
3	E	1003	SAH	C2-N3	2.10	1.35	1.32
3	H	1003	SAH	C2'-C1'	2.10	1.57	1.53
3	B	1003	SAH	C2-N3	2.11	1.35	1.32
3	H	1003	SAH	C2-N3	2.12	1.35	1.32
3	F	1003	SAH	C2-N3	2.14	1.35	1.32
3	C	1003	SAH	C2-N3	2.19	1.36	1.32
3	B	1003	SAH	C2'-C1'	2.20	1.57	1.53
3	A	1003	SAH	C2'-C1'	2.27	1.57	1.53
3	C	1003	SAH	C2'-C1'	2.82	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1003	SAH	C5'-C4'-C3'	-2.13	109.46	114.98
3	F	1003	SAH	C5'-C4'-C3'	-2.00	109.79	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1003	SAH	1	0

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, 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	849/905 (93%)	-0.26	0 100 100	72, 85, 130, 207	0
1	B	851/905 (94%)	-0.18	2 (0%) 95 92	75, 86, 123, 201	0
1	C	852/905 (94%)	-0.19	1 (0%) 95 94	72, 87, 142, 187	0
1	D	848/905 (93%)	-0.24	1 (0%) 95 94	72, 83, 115, 232	0
1	E	852/905 (94%)	-0.13	8 (0%) 85 75	78, 101, 142, 188	0
1	F	850/905 (93%)	-0.23	0 100 100	74, 93, 116, 173	0
1	G	847/905 (93%)	-0.22	2 (0%) 95 92	77, 97, 116, 189	0
1	H	767/905 (84%)	-0.06	12 (1%) 74 61	93, 122, 171, 211	0
All	All	6716/7240 (92%)	-0.19	26 (0%) 93 88	72, 93, 140, 232	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	783	VAL	3.5
1	H	751	THR	3.3
1	E	744	ALA	3.3
1	E	748	LEU	3.1
1	B	578	LYS	2.7
1	H	870	VAL	2.5
1	H	766	TYR	2.5
1	H	872	SER	2.4
1	H	755	GLY	2.3
1	H	345	THR	2.3
1	H	442	LYS	2.3
1	E	874	ILE	2.3
1	E	413	THR	2.2
1	B	411	VAL	2.2
1	C	184	PRO	2.2
1	G	790	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	290	THR	2.2
1	D	723	LYS	2.2
1	H	189	VAL	2.1
1	H	869	GLN	2.1
1	E	794	THR	2.1
1	G	792	ARG	2.1
1	E	745	GLY	2.1
1	H	423	ALA	2.1
1	H	421	ALA	2.0
1	E	752	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	SAH	H	1003	26/26	0.88	0.40	2.16	96,106,159,164	0
3	SAH	G	1003	26/26	0.92	0.35	1.27	94,98,143,184	0
3	SAH	D	1003	26/26	0.94	0.27	0.94	71,72,124,177	0
3	SAH	C	1003	26/26	0.92	0.22	0.07	88,110,137,210	0
2	ZN	G	1001	1/1	0.98	0.23	0.05	98,98,98,98	0
3	SAH	B	1003	26/26	0.92	0.23	-0.11	77,79,94,100	0
2	ZN	C	1001	1/1	0.98	0.18	-0.23	82,82,82,82	0
3	SAH	E	1003	26/26	0.93	0.24	-0.39	93,96,103,171	0
2	ZN	F	1001	1/1	0.99	0.18	-0.51	84,84,84,84	0
3	SAH	F	1003	26/26	0.92	0.19	-0.55	76,83,114,118	0
3	SAH	A	1003	26/26	0.95	0.18	-0.76	78,79,92,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	E	1001	1/1	0.97	0.13	-0.92	100,100,100,100	0
2	ZN	D	1002	1/1	0.99	0.14	-1.08	82,82,82,82	0
2	ZN	E	1002	1/1	0.99	0.08	-1.15	79,79,79,79	0
2	ZN	G	1002	1/1	0.99	0.10	-1.27	84,84,84,84	0
2	ZN	F	1002	1/1	0.98	0.15	-1.29	99,99,99,99	0
2	ZN	B	1001	1/1	0.99	0.15	-1.42	90,90,90,90	0
2	ZN	C	1002	1/1	0.99	0.10	-1.56	76,76,76,76	0
2	ZN	H	1001	1/1	0.96	0.07	-1.66	99,99,99,99	0
2	ZN	A	1001	1/1	0.99	0.06	-1.85	75,75,75,75	0
2	ZN	B	1002	1/1	0.99	0.12	-1.98	77,77,77,77	0
2	ZN	D	1001	1/1	0.98	0.11	-2.18	83,83,83,83	0
2	ZN	A	1002	1/1	0.93	0.06	-2.61	101,101,101,101	0
2	ZN	H	1002	1/1	0.91	0.17	-	146,146,146,146	0

6.5 Other polymers

There are no such residues in this entry.