Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2016 – 08:33 AM EDT

PDB ID	:	5EGS
Title	:	Human PRMT6 with bound fragment-type inhibitor
Authors	:	Steuber, H.; Egner, U.; Kania, J.; Wu, H.; Brown, P.J.
Deposited on	:	2015-10-27
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

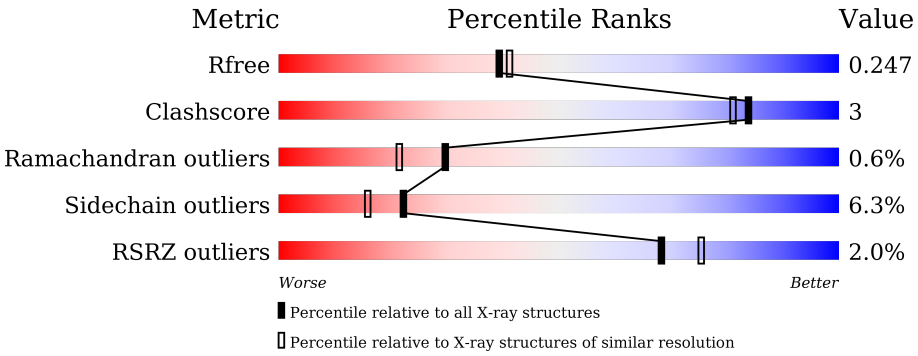
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	376	2% 76% 11% • 11%
1	B	376	79% 10% • 10%
1	C	376	2% 78% 9% •• 10%
1	D	376	2% 77% 10% • 11%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5NR	A	402	-	-	-	X
3	5NR	B	402	-	-	-	X
3	5NR	C	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11269 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.

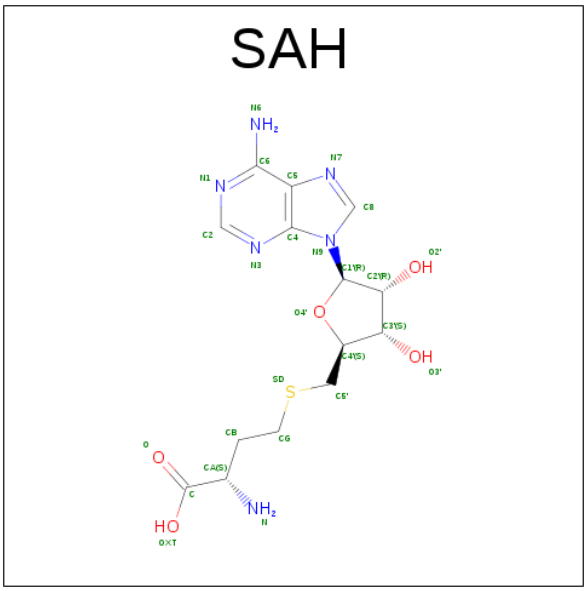
- Molecule 1 is a protein called Protein arginine N-methyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2645	1677	467	487	14			
1	B	338	Total	C	N	O	S	0	1	0
			2687	1700	476	497	14			
1	C	337	Total	C	N	O	S	0	2	0
			2681	1701	470	496	14			
1	D	334	Total	C	N	O	S	0	1	0
			2651	1680	468	489	14			

There are 8 discrepancies between the modelled and reference sequences:

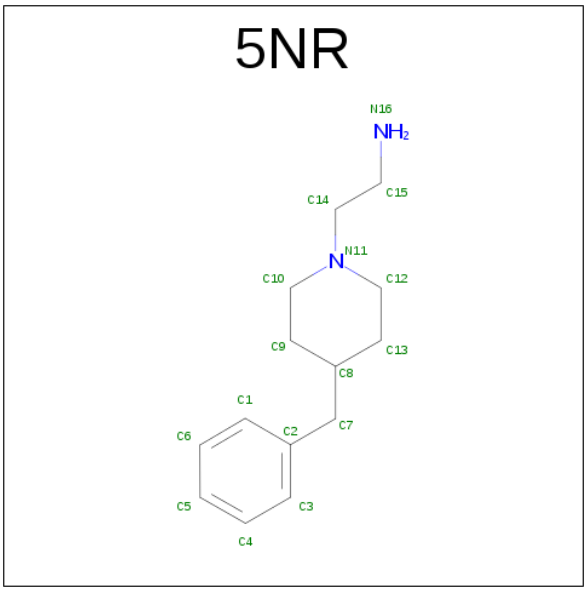
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q96LA8
A	194	VAL	ALA	conflict	UNP Q96LA8
B	0	GLY	-	expression tag	UNP Q96LA8
B	194	VAL	ALA	conflict	UNP Q96LA8
C	0	GLY	-	expression tag	UNP Q96LA8
C	194	VAL	ALA	conflict	UNP Q96LA8
D	0	GLY	-	expression tag	UNP Q96LA8
D	194	VAL	ALA	conflict	UNP Q96LA8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 2-[4-(phenylmethyl)piperidin-1-yl]ethanamine (three-letter code: 5NR) (formula: $C_{14}H_{22}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 16 14 2	0	0
3	A	1	Total C N 16 14 2	0	0
3	B	1	Total C N 16 14 2	0	0
3	C	1	Total C N 16 14 2	0	0
3	C	1	Total C N 16 14 2	0	0
3	D	1	Total C N 16 14 2	0	0

- Molecule 4 is water.

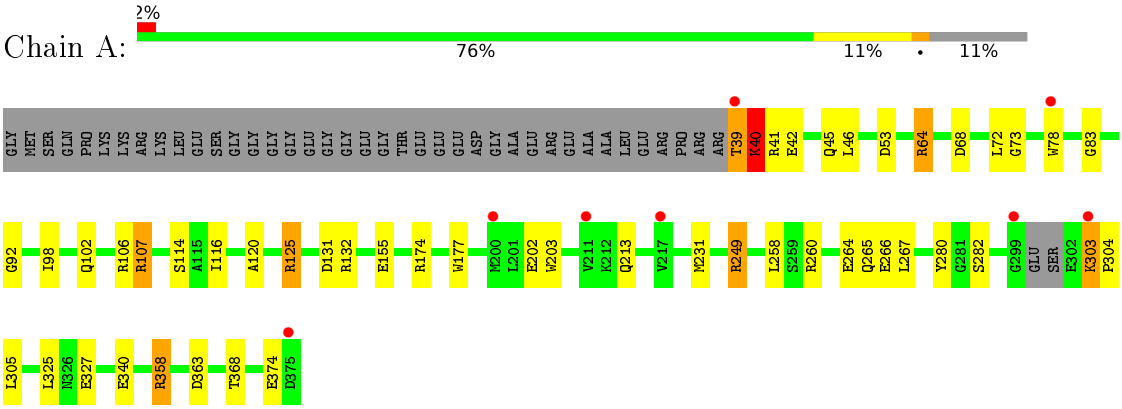
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	110	Total O 110 110	0	0
4	B	119	Total O 119 119	0	0
4	C	85	Total O 85 85	0	0
4	D	91	Total O 91 91	0	0

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.

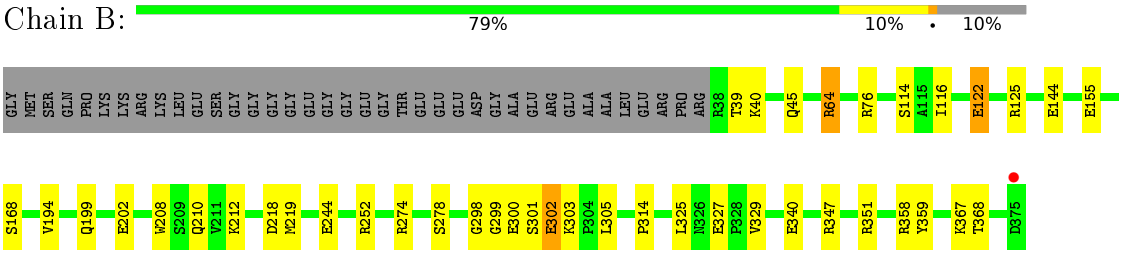
- Molecule 1: Protein arginine N-methyltransferase 6

Chain A:



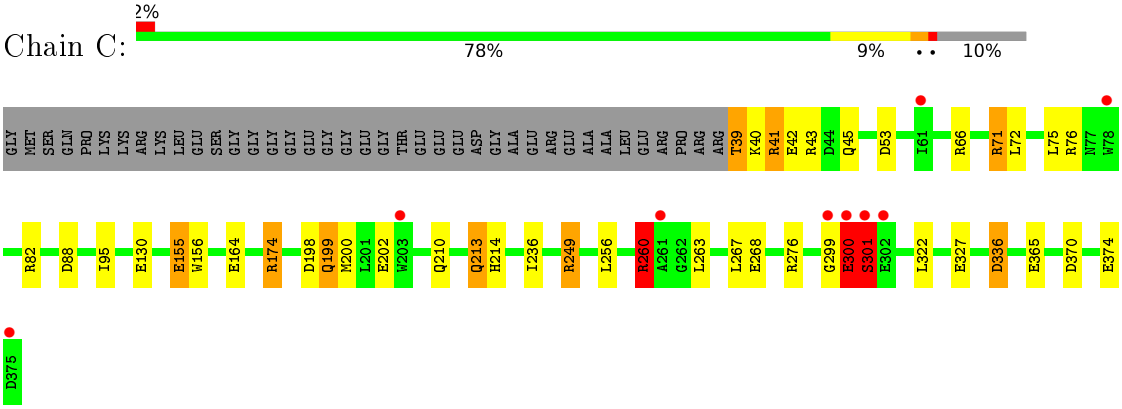
- Molecule 1: Protein arginine N-methyltransferase 6

Chain B:



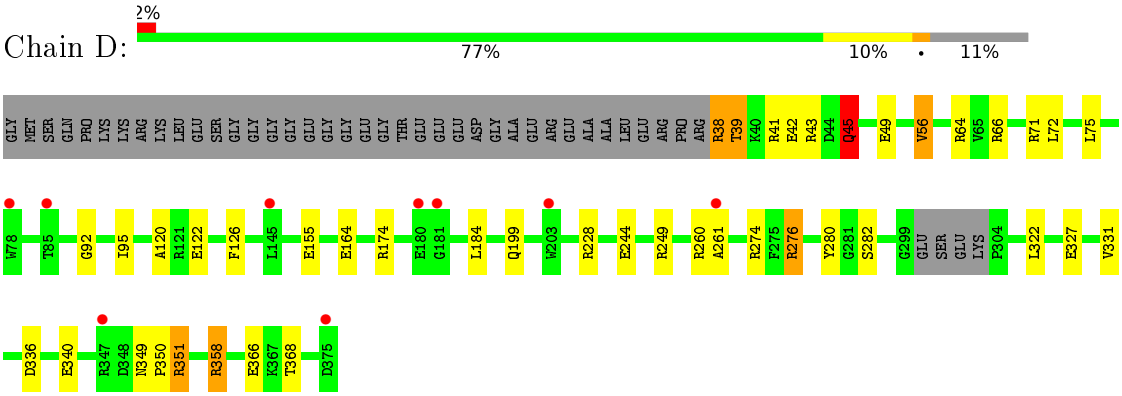
- Molecule 1: Protein arginine N-methyltransferase 6

Chain C:



- Molecule 1: Protein arginine N-methyltransferase 6

Chain D:


2%
77%
10%
11%
GLY MET SER GLN PRO LYS LYS ARG LYS LEU GLU SER GLY GLY GLY GLY GLU GLY GLU GLU GLY THR GLU GLU GLU ASP GLY ALA GLU ARG GLU ALA ALA LEU GLU ARG PRO ARG R38 T39 K40 R41 E42 R43 D44 Q45 E49 V56 R64 V65 R66 R71 L72 L75
W78 T85 G92 I95 A120 R121 E122 F126 L145 E155 E164 R174 E180 G181 L184 Q199 W203 R228 E244 R249 R260 A261 R274 F275 R276 Y280 G281 S282 G299 GLU SER GLU LYS P304 L322 E327 V331
D336 E340 R347 D348 N349 P350 R351 R358 E366 K367 T368 D375

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.16Å 135.62Å 83.09Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	41.26 – 2.15 41.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.26-2.15) 99.3 (41.26-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.201 , 0.246 0.207 , 0.247	Depositor DCC
R_{free} test set	2101 reflections (2.38%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11269	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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: 5NR, 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	1.11	6/2704 (0.2%)	1.14	15/3662 (0.4%)
1	B	1.15	3/2750 (0.1%)	1.12	10/3723 (0.3%)
1	C	1.07	2/2749 (0.1%)	1.14	20/3725 (0.5%)
1	D	1.07	3/2713 (0.1%)	1.11	14/3674 (0.4%)
All	All	1.10	14/10916 (0.1%)	1.13	59/14784 (0.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	GLU	CD-OE2	7.22	1.33	1.25
1	D	280	TYR	CG-CD2	-7.18	1.29	1.39
1	B	368	THR	CB-CG2	-6.63	1.30	1.52
1	B	340	GLU	CD-OE1	-6.61	1.18	1.25
1	D	340	GLU	CD-OE1	-5.77	1.19	1.25
1	A	202	GLU	CD-OE1	5.72	1.31	1.25
1	C	156	TRP	CB-CG	5.52	1.60	1.50
1	A	177	TRP	CB-CG	5.46	1.60	1.50
1	A	282	SER	CB-OG	-5.46	1.35	1.42
1	D	244	GLU	CD-OE2	5.43	1.31	1.25
1	A	78	TRP	CB-CG	5.35	1.59	1.50
1	A	73	GLY	N-CA	5.04	1.53	1.46
1	A	280	TYR	CG-CD1	5.04	1.45	1.39
1	C	155	GLU	CD-OE2	5.01	1.31	1.25

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	D	260	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	B	64	ARG	NE-CZ-NH1	9.10	124.85	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	107	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	C	41	ARG	NE-CZ-NH2	8.97	124.79	120.30
1	C	88	ASP	CB-CG-OD1	8.61	126.05	118.30
1	D	351	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	C	198	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	64	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	252	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	174	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	64	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	B	351	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	370	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	C	370	ASP	CB-CG-OD2	7.31	124.88	118.30
1	D	228	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	64	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	125	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	131	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	274	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	64	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	C	174	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	C	249	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	C	301	SER	N-CA-C	-6.15	94.40	111.00
1	D	56	VAL	CB-CA-C	-6.06	99.89	111.40
1	D	351	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	88	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	249	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	C	41	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	202	GLU	CG-CD-OE1	-5.67	106.96	118.30
1	C	276	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	132	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	174	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	66	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	340	GLU	OE1-CD-OE2	-5.46	116.74	123.30
1	C	41	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	322	LEU	CB-CG-CD1	5.39	120.17	111.00
1	D	274	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	D	71	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	125	ARG	CD-NE-CZ	5.30	131.02	123.60
1	B	218	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	53	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	C	76	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	41	ARG	NE-CZ-NH1	5.22	122.91	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	64	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	66	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	329	VAL	CB-CA-C	-5.15	101.61	111.40
1	B	274	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	D	276	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	363	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	45	GLN	CB-CA-C	5.06	120.52	110.40
1	A	358	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	D	56	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	A	53	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	252	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	C	336	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	71	ARG	NE-CZ-NH2	5.00	122.80	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	2645	0	2603	19	0
1	B	2687	0	2649	13	0
1	C	2681	0	2635	19	0
1	D	2651	0	2612	15	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	32	0	44	4	0
3	B	16	0	22	0	0
3	C	32	0	44	1	0
3	D	16	0	22	0	0
4	A	110	0	0	0	0
4	B	119	0	0	1	0
4	C	85	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	91	0	0	1	0
All	All	11269	0	10707	64	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 (64) 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:C:40:LYS:NZ	4:C:501:HOH:O	1.99	0.93
1:B:122:GLU:OE1	1:B:125:ARG:NH1	2.08	0.86
1:A:39:THR:O	1:A:40:LYS:HB2	1.78	0.82
1:C:260:ARG:HH21	1:C:260:ARG:HG3	1.45	0.82
1:D:39:THR:HG23	1:D:42:GLU:H	1.49	0.78
1:D:351:ARG:NH1	4:D:501:HOH:O	2.08	0.77
1:A:39:THR:HG21	1:A:42:GLU:OE1	1.88	0.73
1:A:114:SER:HB3	1:A:116:ILE:HG22	1.71	0.71
1:D:39:THR:HG22	1:D:42:GLU:CD	2.12	0.70
1:D:39:THR:HG22	1:D:42:GLU:OE1	1.91	0.70
1:A:40:LYS:C	1:A:40:LYS:HD3	2.12	0.69
1:A:83:GLY:O	1:A:106:ARG:NH1	2.28	0.66
1:B:114:SER:HB3	1:B:116:ILE:HG22	1.77	0.66
1:B:219:MET:HE3	1:C:95:ILE:HD12	1.77	0.65
1:C:299:GLY:O	1:C:300:GLU:HB2	1.97	0.64
1:C:213:GLN:HG2	1:D:72:LEU:HD11	1.78	0.64
1:A:267:LEU:HD23	3:A:403:5NR:H9	1.80	0.63
1:B:298:GLY:O	4:B:501:HOH:O	2.15	0.63
1:B:219:MET:CE	1:C:95:ILE:HD12	2.30	0.62
1:A:267:LEU:HB3	3:A:403:5NR:H8	1.80	0.61
1:B:76:ARG:O	1:B:299:GLY:HA3	2.00	0.61
1:C:39:THR:HG23	1:C:42:GLU:OE2	2.01	0.60
1:A:340:GLU:OE2	1:A:358:ARG:NH2	2.35	0.59
1:D:39:THR:CG2	1:D:42:GLU:CG	2.83	0.57
1:A:40:LYS:HD3	1:A:40:LYS:O	2.05	0.57
1:C:260:ARG:NH2	1:C:260:ARG:HG3	2.16	0.57
1:A:98:ILE:O	1:A:102:GLN:HG3	2.05	0.56
1:D:174:ARG:HD2	1:D:184:LEU:HD11	1.88	0.55
1:C:71:ARG:O	1:C:75:LEU:HG	2.09	0.53
1:A:265:GLN:O	1:A:266:GLU:C	2.46	0.53
1:C:260:ARG:HH21	1:C:260:ARG:CG	2.15	0.52
1:B:199:GLN:HG3	1:B:244:GLU:HG3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:NH2	1:C:214:HIS:CD2	2.79	0.50
1:D:39:THR:CG2	1:D:42:GLU:HG3	2.43	0.49
1:C:200:MET:HA	1:C:200:MET:CE	2.43	0.49
1:B:302:GLU:OE2	1:B:303:LYS:N	2.47	0.48
1:D:39:THR:HG22	1:D:42:GLU:CG	2.44	0.47
1:C:199:GLN:HG3	4:C:504:HOH:O	2.14	0.47
1:A:203:TRP:CZ2	1:B:314:PRO:HD3	2.51	0.46
1:C:263:LEU:HG	1:C:267:LEU:HD22	1.97	0.46
1:B:39:THR:CG2	1:B:40:LYS:N	2.78	0.45
1:B:208:TRP:HB3	1:B:219:MET:O	2.16	0.45
1:D:45:GLN:NE2	1:D:49[A]:GLU:OE2	2.50	0.44
1:A:231:MET:HB3	1:A:325:LEU:O	2.17	0.44
1:D:38:ARG:N	1:D:38:ARG:HH11	2.15	0.44
1:C:236:ILE:O	1:C:374:GLU:HB2	2.19	0.43
1:A:40:LYS:CD	1:A:40:LYS:C	2.86	0.43
1:D:349:ASN:HA	1:D:350:PRO:HD2	1.91	0.43
1:C:260:ARG:NH2	1:C:260:ARG:CG	2.73	0.43
1:D:92:GLY:O	1:D:120:ALA:HB2	2.19	0.43
1:A:303:LYS:CB	1:A:304:PRO:CD	2.97	0.42
1:A:305:LEU:C	1:A:305:LEU:HD23	2.40	0.42
1:D:358:ARG:NH2	1:D:366:GLU:OE2	2.48	0.42
3:C:403:5NR:H22	3:C:403:5NR:H13	1.84	0.42
1:C:43:ARG:NE	4:C:503:HOH:O	2.38	0.42
1:C:256:LEU:N	1:C:256:LEU:HD12	2.35	0.41
3:A:403:5NR:H22	3:A:403:5NR:H13	1.85	0.41
1:A:64:ARG:O	1:A:68:ASP:HB2	2.21	0.41
1:B:325:LEU:HD22	1:B:359:TYR:CZ	2.55	0.41
1:C:39:THR:N	1:C:42:GLU:OE2	2.54	0.41
1:A:92:GLY:O	1:A:120:ALA:HB2	2.21	0.41
3:A:402:5NR:C3	3:A:402:5NR:H10	2.48	0.40
1:A:303:LYS:HB3	1:A:304:PRO:HD3	2.03	0.40
1:D:282:SER:HA	1:D:331:VAL:O	2.20	0.40

There are no symmetry-related clashes.

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	331/376 (88%)	320 (97%)	9 (3%)	2 (1%)	30 21
1	B	337/376 (90%)	329 (98%)	8 (2%)	0	100 100
1	C	337/376 (90%)	321 (95%)	12 (4%)	4 (1%)	16 9
1	D	331/376 (88%)	319 (96%)	10 (3%)	2 (1%)	30 21
All	All	1336/1504 (89%)	1289 (96%)	39 (3%)	8 (1%)	30 21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	C	260	ARG
1	C	300	GLU
1	C	301	SER
1	D	261	ALA
1	C	164	GLU
1	D	164	GLU
1	A	374	GLU

5.3.2 Protein sidechains (i)

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	279/310 (90%)	264 (95%)	15 (5%)	27 22
1	B	285/310 (92%)	268 (94%)	17 (6%)	24 18
1	C	284/310 (92%)	264 (93%)	20 (7%)	19 12
1	D	281/310 (91%)	262 (93%)	19 (7%)	20 13
All	All	1129/1240 (91%)	1058 (94%)	71 (6%)	22 16

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	40	LYS
1	A	45	GLN
1	A	46	LEU
1	A	72	LEU
1	A	107	ARG
1	A	125	ARG
1	A	155	GLU
1	A	213	GLN
1	A	249	ARG
1	A	258	LEU
1	A	264	GLU
1	A	303	LYS
1	A	327	GLU
1	A	368	THR
1	B	45	GLN
1	B	122	GLU
1	B	144	GLU
1	B	155	GLU
1	B	168	SER
1	B	194	VAL
1	B	210	GLN
1	B	212	LYS
1	B	278	SER
1	B	300	GLU
1	B	301	SER
1	B	302	GLU
1	B	305	LEU
1	B	327	GLU
1	B	347	ARG
1	B	358	ARG
1	B	367	LYS
1	C	39	THR
1	C	41	ARG
1	C	45	GLN
1	C	72	LEU
1	C	82	ARG
1	C	130	GLU
1	C	155	GLU
1	C	174	ARG
1	C	199	GLN
1	C	202	GLU
1	C	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	213	GLN
1	C	249	ARG
1	C	260	ARG
1	C	268	GLU
1	C	300	GLU
1	C	301	SER
1	C	327	GLU
1	C	336	ASP
1	C	365	GLU
1	D	38	ARG
1	D	39	THR
1	D	41	ARG
1	D	43	ARG
1	D	45	GLN
1	D	56	VAL
1	D	75	LEU
1	D	95	ILE
1	D	122	GLU
1	D	126	PHE
1	D	155	GLU
1	D	199	GLN
1	D	249	ARG
1	D	276	ARG
1	D	322	LEU
1	D	327	GLU
1	D	336	ASP
1	D	358	ARG
1	D	368	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	B	45	GLN
1	B	210	GLN
1	C	214	HIS
1	C	364	GLN
1	D	45	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

10 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	$\#\|Z\| > 2$
2	SAH	A	401	-	22,28,28	1.04	1 (4%)	18,40,40	2.08	3 (16%)
3	5NR	A	402	-	17,17,17	0.62	0	21,21,21	1.55	3 (14%)
3	5NR	A	403	-	17,17,17	0.93	0	21,21,21	1.35	4 (19%)
2	SAH	B	401	-	22,28,28	0.91	0	18,40,40	2.42	4 (22%)
3	5NR	B	402	-	17,17,17	0.74	0	21,21,21	1.25	1 (4%)
2	SAH	C	401	-	22,28,28	1.03	2 (9%)	18,40,40	2.66	4 (22%)
3	5NR	C	402	-	17,17,17	0.76	0	21,21,21	1.17	2 (9%)
3	5NR	C	403	-	17,17,17	0.75	0	21,21,21	1.22	3 (14%)
2	SAH	D	401	-	22,28,28	1.24	3 (13%)	18,40,40	2.79	4 (22%)
3	5NR	D	402	-	17,17,17	0.90	0	21,21,21	0.64	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
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
3	5NR	A	402	-	-	0/7/17/17	0/2/2/2
3	5NR	A	403	-	-	0/7/17/17	0/2/2/2
2	SAH	B	401	-	-	0/7/31/31	0/3/3/3
3	5NR	B	402	-	-	0/7/17/17	0/2/2/2
2	SAH	C	401	-	-	0/7/31/31	0/3/3/3
3	5NR	C	402	-	-	0/7/17/17	0/2/2/2
3	5NR	C	403	-	-	0/7/17/17	0/2/2/2
2	SAH	D	401	-	-	0/7/31/31	0/3/3/3
3	5NR	D	402	-	-	0/7/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	SAH	C2'-C1'	-2.40	1.49	1.53
2	D	401	SAH	C5-C4	2.46	1.46	1.40
2	C	401	SAH	C5-C4	2.59	1.46	1.40
2	C	401	SAH	C2-N3	2.73	1.37	1.32
2	D	401	SAH	C2-N3	2.82	1.37	1.32
2	A	401	SAH	C5-C4	2.93	1.47	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	SAH	N3-C2-N1	-10.11	120.93	128.87
2	D	401	SAH	N3-C2-N1	-9.66	121.28	128.87
2	B	401	SAH	N3-C2-N1	-8.67	122.06	128.87
2	A	401	SAH	N3-C2-N1	-7.16	123.24	128.87
2	D	401	SAH	C1'-N9-C4	-4.22	122.09	126.81
3	A	402	5NR	C2-C7-C8	-3.51	109.20	114.68
3	B	402	5NR	C14-C15-N16	-3.44	102.16	112.91
3	A	403	5NR	C14-N11-C10	-2.91	104.90	111.25
3	A	403	5NR	C5-C6-C1	-2.81	116.30	120.20
2	A	401	SAH	C1'-N9-C4	-2.64	123.86	126.81
3	C	403	5NR	C5-C6-C1	-2.53	116.69	120.20
3	A	402	5NR	C9-C8-C7	-2.41	106.30	111.86
2	B	401	SAH	C1'-N9-C4	-2.35	124.18	126.81
3	C	403	5NR	C14-N11-C10	-2.13	106.60	111.25
3	C	403	5NR	C2-C7-C8	-2.11	111.39	114.68
3	C	402	5NR	C13-C8-C7	-2.04	107.14	111.86
3	A	403	5NR	C9-C10-N11	2.01	114.33	110.97
2	A	401	SAH	C4'-O4'-C1'	2.04	111.81	109.64
3	A	403	5NR	C12-C13-C8	2.11	115.44	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	SAH	C2-N1-C6	2.11	122.54	118.77
2	C	401	SAH	C2'-C1'-N9	2.14	119.20	113.47
2	C	401	SAH	C4'-O4'-C1'	2.20	111.97	109.64
2	B	401	SAH	C2'-C3'-C4'	2.25	107.24	102.64
3	C	402	5NR	C10-C9-C8	2.28	115.74	111.85
2	D	401	SAH	N6-C6-N1	2.55	122.80	118.52
2	C	401	SAH	N6-C6-N1	2.57	122.83	118.52
2	B	401	SAH	N6-C6-N1	2.87	123.33	118.52
3	A	402	5NR	C10-C9-C8	3.84	118.40	111.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	5NR	1	0
3	A	403	5NR	3	0
3	C	403	5NR	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	335/376 (89%)	0.10	8 (2%)	62	71	16, 31, 50, 68	5 (1%)
1	B	338/376 (89%)	-0.01	1 (0%)	94	95	14, 26, 46, 72	1 (0%)
1	C	337/376 (89%)	0.16	9 (2%)	58	67	18, 29, 54, 87	6 (1%)
1	D	334/376 (88%)	0.12	9 (2%)	58	67	19, 32, 53, 67	5 (1%)
All	All	1344/1504 (89%)	0.09	27 (2%)	68	75	14, 29, 52, 87	17 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	SER	4.9
1	A	303	LYS	4.8
1	C	300	GLU	4.6
1	C	61	ILE	3.5
1	A	78	TRP	3.2
1	D	180	GLU	3.1
1	D	85	THR	3.0
1	C	299	GLY	3.0
1	D	375	ASP	3.0
1	D	145	LEU	3.0
1	A	375	ASP	2.9
1	C	261	ALA	2.7
1	B	375	ASP	2.7
1	A	200	MET	2.7
1	C	375	ASP	2.6
1	A	39	THR	2.5
1	D	181	GLY	2.5
1	A	299	GLY	2.5
1	D	347	ARG	2.4
1	D	203	TRP	2.3
1	C	302	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	203[A]	TRP	2.1
1	D	78	TRP	2.1
1	A	217	VAL	2.1
1	A	211	VAL	2.0
1	C	78	TRP	2.0
1	D	261	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	5NR	B	402	16/16	0.86	0.17	5.42	16,19,25,26	0
3	5NR	A	402	16/16	0.94	0.14	3.67	15,20,27,28	0
3	5NR	C	402	16/16	0.91	0.17	2.60	19,22,34,35	0
3	5NR	C	403	16/16	0.85	0.21	1.81	32,41,51,51	0
3	5NR	D	402	16/16	0.91	0.13	1.60	16,18,24,24	0
3	5NR	A	403	16/16	0.92	0.16	0.65	25,33,37,37	0
2	SAH	B	401	26/26	0.97	0.11	0.19	15,19,21,23	0
2	SAH	C	401	26/26	0.96	0.11	-0.27	18,20,23,24	0
2	SAH	A	401	26/26	0.96	0.10	-0.42	18,22,23,24	0
2	SAH	D	401	26/26	0.95	0.11	-0.57	21,25,27,29	0

6.5 Other polymers (i)

There are no such residues in this entry.