



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:26 pm GMT

PDB ID : 2B4Y  
Title : Crystal Structure of Human Sirtuin homolog 5  
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Deposited on : 2005-09-27  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

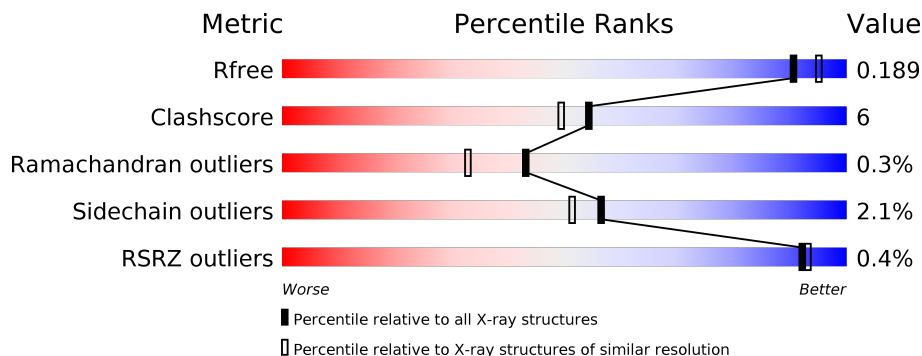
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	<div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	B	271	<div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	C	271	<div> <div>87%</div> <div>10%</div> <div>•</div> </div>
1	D	271	<div> <div>%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8930 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 NAD-dependent deacetylase sirtuin-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	Se	0	0	0
			1992	1257	360	363	9	3			
1	B	262	Total	C	N	O	S	Se	0	0	0
			2006	1266	362	366	9	3			
1	C	263	Total	C	N	O	S	Se	0	0	0
			2011	1270	363	366	9	3			
1	D	262	Total	C	N	O	S	Se	0	0	0
			2006	1267	362	365	9	3			

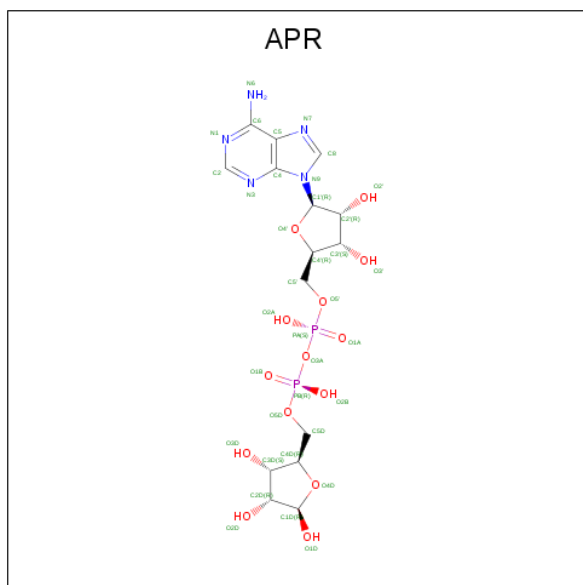
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	CLONING ARTIFACT	UNP Q9NXA8
A	33	SER	-	CLONING ARTIFACT	UNP Q9NXA8
A	40	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
A	259	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
B	32	GLY	-	CLONING ARTIFACT	UNP Q9NXA8
B	33	SER	-	CLONING ARTIFACT	UNP Q9NXA8
B	40	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
B	259	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
C	32	GLY	-	CLONING ARTIFACT	UNP Q9NXA8
C	33	SER	-	CLONING ARTIFACT	UNP Q9NXA8
C	40	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
C	259	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
D	32	GLY	-	CLONING ARTIFACT	UNP Q9NXA8
D	33	SER	-	CLONING ARTIFACT	UNP Q9NXA8
D	40	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8
D	259	MSE	MET	MODIFIED RESIDUE	UNP Q9NXA8

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

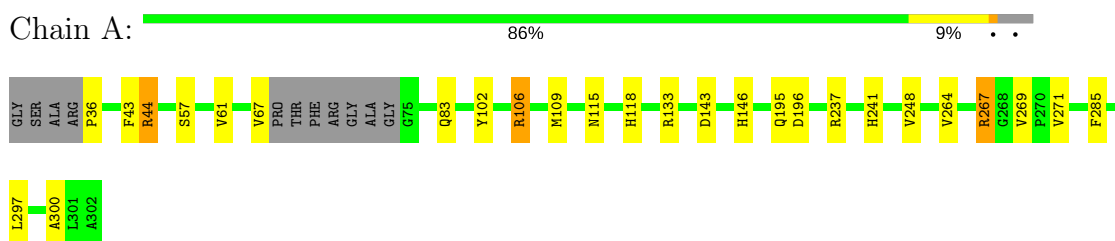
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	191	Total	O	0	0
			191	191		
5	B	192	Total	O	0	0
			192	192		
5	C	176	Total	O	0	0
			176	176		
5	D	148	Total	O	0	0
			148	148		

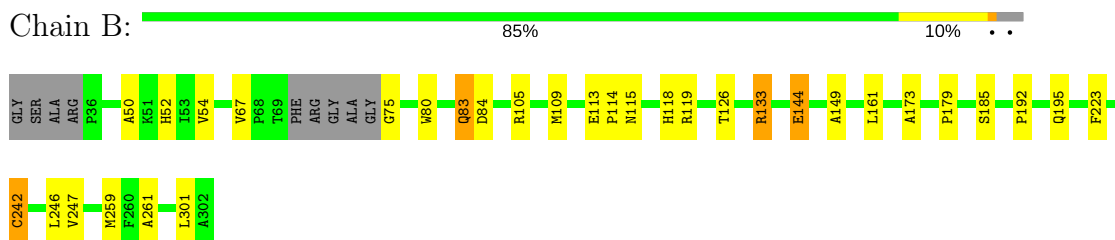
### 3 Residue-property plots [i](#)

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

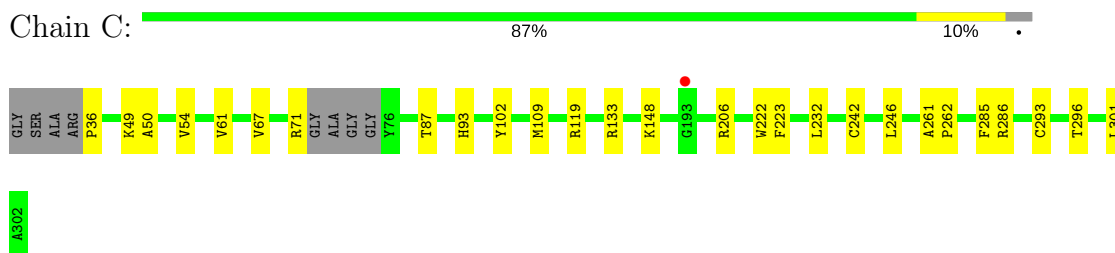
- Molecule 1: NAD-dependent deacetylase sirtuin-5



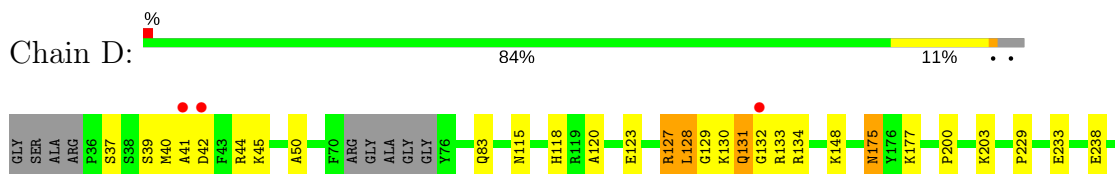
- Molecule 1: NAD-dependent deacetylase sirtuin-5



- Molecule 1: NAD-dependent deacetylase sirtuin-5



- Molecule 1: NAD-dependent deacetylase sirtuin-5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.57Å 58.76Å 104.97Å 93.50° 92.75° 94.98°	Depositor
Resolution (Å)	40.30 – 1.90 40.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.30-1.90) 95.5 (40.30-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.236 0.185 , 0.189	Depositor DCC
$R_{free}$ test set	4024 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APR, ZN, EPE

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	0.93	1/2039 (0.0%)	1.08	9/2761 (0.3%)
1	B	0.89	2/2054 (0.1%)	0.79	2/2783 (0.1%)
1	C	0.90	0/2059	0.84	2/2790 (0.1%)
1	D	0.83	0/2054	0.79	0/2783
All	All	0.89	3/8206 (0.0%)	0.88	13/11117 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	CYS	CB-SG	-5.44	1.73	1.81
1	B	173	ALA	CA-CB	5.10	1.63	1.52
1	A	106	ARG	CD-NE	-5.01	1.38	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ARG	NE-CZ-NH2	-22.67	108.96	120.30
1	A	106	ARG	NE-CZ-NH1	16.77	128.69	120.30
1	A	267	ARG	NE-CZ-NH2	-15.83	112.39	120.30
1	C	206	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	A	267	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	C	206	ARG	NE-CZ-NH1	8.72	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	106	ARG	CG-CD-NE	-6.20	98.78	111.80
1	B	133	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	133	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	143	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	267	ARG	CD-NE-CZ	5.51	131.32	123.60
1	B	133	ARG	NE-CZ-NH1	5.39	122.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	132	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1992	0	1959	23	0
1	B	2006	0	1973	26	0
1	C	2011	0	1974	16	0
1	D	2006	0	1972	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	36	0	21	2	0
3	B	36	0	21	1	0
3	C	36	0	21	0	0
3	D	36	0	21	1	0
4	A	15	0	17	2	0
4	B	15	0	17	5	0
4	C	15	0	17	0	0
4	D	15	0	17	2	0
5	A	191	0	0	6	0
5	B	192	0	0	10	1
5	C	176	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	148	0	0	3	0
All	All	8930	0	8030	93	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 6.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ARG:O	1:D:129:GLY:N	1.88	1.06
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.22	1.00
1:B:144:GLU:HG3	5:B:2168:HOH:O	1.65	0.95
1:B:126:THR:HG22	5:B:2019:HOH:O	1.71	0.89
1:B:115:ASN:H	1:B:118:HIS:HD2	1.23	0.84
1:B:83:GLN:H	1:B:83:GLN:HE21	1.26	0.83
1:D:127:ARG:HG3	1:D:128:LEU:H	1.44	0.82
3:A:1002:APR:O2D	4:A:1003:EPE:H21	1.80	0.81
1:A:115:ASN:H	1:A:118:HIS:HD2	1.26	0.81
1:D:115:ASN:H	1:D:118:HIS:HD2	1.27	0.79
1:A:195:GLN:HG3	1:A:196:ASP:H	1.48	0.78
1:D:200:PRO:HG2	1:D:203:LYS:HD2	1.68	0.76
3:B:2002:APR:O2D	4:B:2003:EPE:H21	1.88	0.73
1:A:195:GLN:HG3	1:A:196:ASP:N	2.06	0.70
1:B:50:ALA:O	1:B:133:ARG:HD2	1.91	0.70
3:D:4002:APR:O2D	4:D:4003:EPE:H21	1.94	0.68
1:D:127:ARG:O	1:D:128:LEU:C	2.31	0.67
1:D:131:GLN:HE21	1:D:133:ARG:HH21	1.43	0.66
1:D:41:ALA:O	1:D:45:LYS:HG2	1.96	0.65
1:C:67:VAL:HG13	1:C:109:MSE:HE1	1.79	0.65
1:C:67:VAL:CG1	1:C:109:MSE:HE1	2.27	0.64
1:A:44:ARG:CG	1:A:44:ARG:HH11	2.06	0.64
1:B:105:ARG:NH2	4:B:2003:EPE:O2S	2.32	0.62
1:A:267:ARG:HD3	5:A:1158:HOH:O	1.99	0.61
1:D:175:ASN:HD21	1:D:177:LYS:HB2	1.66	0.61
1:B:179:PRO:HG3	1:B:185:SER:HB2	1.82	0.61
1:D:127:ARG:O	1:D:130:LYS:N	2.32	0.60
1:A:195:GLN:CG	1:A:196:ASP:H	2.14	0.60
1:A:44:ARG:HG3	1:A:44:ARG:NH1	2.02	0.60
1:B:67:VAL:HG13	1:B:109:MSE:HE1	1.86	0.58
1:B:149:ALA:O	5:B:2183:HOH:O	2.17	0.57
1:D:127:ARG:HG3	1:D:128:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLU:HG2	1:B:114:PRO:HD2	1.87	0.56
1:A:67:VAL:HG13	1:A:109:MSE:HE1	1.88	0.56
1:B:75:GLY:N	5:B:2030:HOH:O	2.39	0.55
1:B:83:GLN:H	1:B:83:GLN:NE2	1.99	0.55
1:B:67:VAL:CG1	1:B:109:MSE:HE1	2.38	0.54
1:D:50:ALA:O	1:D:133:ARG:HD2	2.08	0.53
1:D:40:MSE:O	1:D:44:ARG:HG2	2.09	0.52
1:A:36:PRO:N	5:A:1169:HOH:O	2.43	0.52
1:B:195:GLN:HG2	5:B:2178:HOH:O	2.08	0.52
1:D:131:GLN:HG3	1:D:133:ARG:HE	1.75	0.52
1:C:87:THR:HG22	1:C:223:PHE:HB2	1.91	0.51
1:B:54:VAL:HG23	1:B:242:CYS:HB3	1.92	0.51
1:B:83:GLN:N	1:B:83:GLN:HE21	2.03	0.49
1:C:119:ARG:HD2	5:C:3155:HOH:O	2.12	0.48
1:C:109:MSE:HE2	5:C:3151:HOH:O	2.12	0.48
1:C:71:ARG:CB	5:C:3148:HOH:O	2.61	0.48
1:A:264:VAL:HG12	1:A:269:VAL:HB	1.96	0.48
1:C:54:VAL:HG23	1:C:242:CYS:HB3	1.96	0.47
3:A:1002:APR:HOR2	4:A:1003:EPE:H21	1.76	0.47
1:A:115:ASN:H	1:A:118:HIS:CD2	2.17	0.47
1:D:45:LYS:HA	5:D:4130:HOH:O	2.14	0.47
1:A:146:HIS:HD2	5:A:1012:HOH:O	1.96	0.47
1:A:248:VAL:HG11	1:A:297:LEU:HD11	1.96	0.47
1:D:120:ALA:HA	1:D:123:GLU:HG2	1.97	0.46
1:A:106:ARG:HD3	5:A:1006:HOH:O	2.16	0.46
1:A:237:ARG:O	1:A:241:HIS:HD2	1.98	0.45
1:A:43:PHE:CE2	1:A:300:ALA:HB1	2.51	0.45
1:B:144:GLU:CG	5:B:2168:HOH:O	2.39	0.45
1:C:102:TYR:HH	1:C:222:TRP:HE1	1.64	0.45
1:C:50:ALA:O	1:C:133:ARG:HD2	2.17	0.45
1:A:44:ARG:NH1	1:A:44:ARG:CG	2.73	0.45
1:D:39:SER:HB3	1:D:42:ASP:HB2	1.99	0.45
1:A:237:ARG:NH2	5:A:1069:HOH:O	2.50	0.44
1:D:134:ARG:NH2	1:D:238:GLU:OE2	2.45	0.44
1:B:259:MSE:HB2	5:B:2163:HOH:O	2.18	0.44
1:D:256:PRO:HD2	5:D:4013:HOH:O	2.18	0.44
1:A:237:ARG:NE	5:A:1069:HOH:O	2.50	0.43
1:B:223:PHE:CZ	4:B:2003:EPE:H61	2.53	0.43
1:A:102:TYR:O	1:A:106:ARG:HG3	2.17	0.43
5:B:2048:HOH:O	1:D:45:LYS:HE3	2.17	0.43
1:B:109:MSE:HG3	1:B:161:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:VAL:HG11	1:C:109:MSE:HE1	1.99	0.43
1:A:57:SER:OG	1:A:146:HIS:HE1	2.02	0.43
1:C:261:ALA:HB3	1:C:262:PRO:HD3	2.00	0.43
1:D:229:PRO:O	1:D:233:GLU:HG3	2.19	0.43
4:B:2003:EPE:H22	4:B:2003:EPE:H101	1.92	0.43
1:B:119:ARG:HD3	5:B:2183:HOH:O	2.19	0.43
1:B:192:PRO:HA	5:B:2189:HOH:O	2.18	0.43
1:B:105:ARG:NH1	4:B:2003:EPE:O2S	2.52	0.43
1:B:246:LEU:HD21	1:B:301:LEU:HD21	2.01	0.43
1:C:54:VAL:HG23	1:C:242:CYS:CB	2.49	0.42
1:A:271:VAL:HG11	1:A:285:PHE:CD1	2.54	0.42
1:C:36:PRO:N	5:C:3169:HOH:O	2.53	0.42
4:D:4003:EPE:H52	5:D:4125:HOH:O	2.20	0.42
1:B:247:VAL:HG21	1:B:261:ALA:CB	2.50	0.41
1:C:36:PRO:HB3	1:C:285:PHE:O	2.20	0.41
1:D:275:ASN:O	1:D:290:GLN:HA	2.20	0.41
1:C:293:CYS:HA	1:C:296:THR:OG1	2.21	0.41
1:C:246:LEU:HD21	1:C:301:LEU:HD21	2.03	0.41
1:B:80:TRP:HB3	1:B:84:ASP:HB2	2.04	0.41
1:D:175:ASN:ND2	1:D:177:LYS:H	2.19	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)
5:B:2161:HOH:O	5:B:2186:HOH:O[1_455]	2.04	0.16

## 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	256/271 (94%)	254 (99%)	2 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	258/271 (95%)	254 (98%)	4 (2%)	0	100	100
1	C	259/271 (96%)	254 (98%)	5 (2%)	0	100	100
1	D	258/271 (95%)	250 (97%)	5 (2%)	3 (1%)	14	5
All	All	1031/1084 (95%)	1012 (98%)	16 (2%)	3 (0%)	43	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	127	ARG
1	D	128	LEU
1	D	131	GLN

### 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	209/212 (99%)	206 (99%)	3 (1%)	69	67
1	B	211/212 (100%)	208 (99%)	3 (1%)	69	67
1	C	211/212 (100%)	205 (97%)	6 (3%)	47	39
1	D	211/212 (100%)	205 (97%)	6 (3%)	47	39
All	All	842/848 (99%)	824 (98%)	18 (2%)	56	51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	61	VAL
1	A	83	GLN
1	B	52	HIS
1	B	83	GLN
1	B	144	GLU
1	C	49	LYS
1	C	61	VAL

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Mol	Chain	Res	Type
1	C	93	HIS
1	C	148	LYS
1	C	232	LEU
1	C	286	ARG
1	D	37	SER
1	D	83	GLN
1	D	148	LYS
1	D	175	ASN
1	D	264	VAL
1	D	276	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	118	HIS
1	A	140	GLN
1	A	146	HIS
1	A	241	HIS
1	A	290	GLN
1	B	83	GLN
1	B	118	HIS
1	B	140	GLN
1	B	290	GLN
1	D	118	HIS
1	D	131	GLN
1	D	175	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 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	APR	A	1002	-	34,39,39	0.95	1 (2%)	38,60,60	1.79	7 (18%)
4	EPE	A	1003	-	15,15,15	1.02	1 (6%)	18,20,20	2.01	5 (27%)
3	APR	B	2002	-	34,39,39	0.95	3 (8%)	38,60,60	2.06	9 (23%)
4	EPE	B	2003	-	15,15,15	0.92	1 (6%)	18,20,20	1.89	6 (33%)
3	APR	C	3002	-	34,39,39	1.33	3 (8%)	38,60,60	2.01	6 (15%)
4	EPE	C	3003	-	15,15,15	0.96	1 (6%)	18,20,20	1.68	4 (22%)
3	APR	D	4002	-	34,39,39	1.17	2 (5%)	38,60,60	2.41	8 (21%)
4	EPE	D	4003	-	15,15,15	1.04	1 (6%)	18,20,20	3.95	10 (55%)

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	APR	A	1002	-	-	0/18/54/54	0/4/4/4
4	EPE	A	1003	-	-	0/9/19/19	0/1/1/1
3	APR	B	2002	-	-	0/18/54/54	0/4/4/4
4	EPE	B	2003	-	-	0/9/19/19	0/1/1/1
3	APR	C	3002	-	-	0/18/54/54	0/4/4/4
4	EPE	C	3003	-	-	0/9/19/19	0/1/1/1
3	APR	D	4002	-	-	0/18/54/54	0/4/4/4
4	EPE	D	4003	-	-	0/9/19/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	APR	C4-N3	2.10	1.38	1.35
3	B	2002	APR	C2-N3	2.23	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	APR	C2-N3	2.51	1.36	1.32
3	B	2002	APR	C5-C4	2.58	1.46	1.40
3	A	1002	APR	C5-C4	2.75	1.46	1.40
4	B	2003	EPE	C10-S	2.89	1.81	1.77
4	D	4003	EPE	C10-S	3.35	1.82	1.77
4	C	3003	EPE	C10-S	3.36	1.82	1.77
4	A	1003	EPE	C10-S	3.44	1.82	1.77
3	D	4002	APR	C5-C4	3.52	1.48	1.40
3	C	3002	APR	C5-C4	3.60	1.48	1.40
3	C	3002	APR	O4'-C1'	3.90	1.46	1.41
3	D	4002	APR	O4'-C1'	4.31	1.47	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4002	APR	N3-C2-N1	-8.79	121.34	128.86
3	B	2002	APR	N3-C2-N1	-8.73	121.39	128.86
4	D	4003	EPE	O1S-S-C10	-8.53	96.65	106.92
3	A	1002	APR	N3-C2-N1	-7.23	122.68	128.86
3	C	3002	APR	N3-C2-N1	-5.86	123.84	128.86
3	C	3002	APR	C4-C5-N7	-4.55	105.01	109.41
3	C	3002	APR	O2D-C2D-C1D	-4.12	100.48	111.85
3	D	4002	APR	O2D-C2D-C1D	-3.74	101.54	111.85
3	A	1002	APR	O1D-C1D-O4D	-3.63	106.33	111.12
4	D	4003	EPE	C9-N1-C6	-3.62	101.78	111.24
3	B	2002	APR	C1'-N9-C4	-3.56	120.49	126.64
3	D	4002	APR	C4-C5-N7	-3.41	106.11	109.41
3	B	2002	APR	O3'-C3'-C4'	-2.90	102.65	111.06
3	D	4002	APR	C1'-N9-C4	-2.70	121.97	126.64
4	C	3003	EPE	C9-N1-C6	-2.55	104.57	111.24
3	A	1002	APR	C4-C5-N7	-2.26	107.22	109.41
4	B	2003	EPE	C9-N1-C6	-2.26	105.34	111.24
3	A	1002	APR	C1'-N9-C4	-2.25	122.75	126.64
3	D	4002	APR	O4D-C4D-C3D	-2.20	100.79	105.15
3	A	1002	APR	C4'-O4'-C1'	-2.19	107.55	109.83
4	C	3003	EPE	C5-C6-N1	-2.16	106.39	110.64
3	B	2002	APR	O4D-C4D-C3D	-2.14	100.91	105.15
4	A	1003	EPE	C5-C6-N1	-2.12	106.46	110.64
3	B	2002	APR	O2D-C2D-C1D	-2.01	106.30	111.85
3	C	3002	APR	O4D-C4D-C3D	-2.01	101.19	105.15
3	C	3002	APR	O1D-C1D-C2D	2.08	120.70	110.41
3	B	2002	APR	N6-C6-N1	2.08	122.88	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4003	EPE	C3-C2-N1	2.10	114.77	110.64
4	B	2003	EPE	C6-N1-C2	2.22	113.78	108.87
3	A	1002	APR	C1D-C2D-C3D	2.43	105.34	102.30
4	B	2003	EPE	C7-N4-C5	2.44	117.62	111.24
4	D	4003	EPE	C5-C6-N1	2.45	115.47	110.64
3	B	2002	APR	O1D-C1D-O4D	2.50	114.42	111.12
4	B	2003	EPE	C3-C2-N1	2.52	115.60	110.64
4	D	4003	EPE	C6-C5-N4	2.52	115.61	110.64
3	A	1002	APR	O2A-PA-O1A	2.64	125.55	112.14
3	D	4002	APR	O3D-C3D-C4D	2.73	118.96	111.06
3	B	2002	APR	O2A-PA-O1A	2.77	126.21	112.14
4	B	2003	EPE	C7-N4-C3	2.90	118.80	111.24
4	A	1003	EPE	C2-C3-N4	2.98	116.50	110.64
3	D	4002	APR	C2-N1-C6	2.98	123.82	118.75
4	A	1003	EPE	C7-N4-C3	3.10	119.34	111.24
3	B	2002	APR	C2-N1-C6	3.16	124.12	118.75
4	C	3003	EPE	C7-N4-C3	3.36	120.02	111.24
4	A	1003	EPE	C7-N4-C5	3.50	120.39	111.24
4	D	4003	EPE	C2-C3-N4	3.78	118.08	110.64
4	C	3003	EPE	C5-N4-C3	3.95	117.61	108.87
4	B	2003	EPE	C5-N4-C3	4.16	118.07	108.87
4	D	4003	EPE	C6-N1-C2	4.34	118.46	108.87
4	D	4003	EPE	C7-N4-C3	4.96	124.19	111.24
4	A	1003	EPE	C5-N4-C3	5.11	120.18	108.87
4	D	4003	EPE	C5-N4-C3	6.47	123.18	108.87
3	C	3002	APR	O1D-C1D-O4D	6.85	120.16	111.12
3	D	4002	APR	O1D-C1D-O4D	8.00	121.67	111.12
4	D	4003	EPE	O3S-S-C10	8.42	119.38	105.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	APR	2	0
4	A	1003	EPE	2	0
3	B	2002	APR	1	0
4	B	2003	EPE	5	0
3	D	4002	APR	1	0
4	D	4003	EPE	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/271 (94%)	-0.31	0	100 100	14, 22, 32, 40	0
1	B	259/271 (95%)	-0.29	0	100 100	15, 23, 32, 40	0
1	C	260/271 (95%)	-0.24	1 (0%)	92 93	15, 25, 36, 40	0
1	D	259/271 (95%)	-0.09	3 (1%)	79 81	15, 26, 44, 51	0
All	All	1035/1084 (95%)	-0.23	4 (0%)	92 93	14, 24, 37, 51	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	ALA	3.1
1	D	42	ASP	2.8
1	C	193	GLY	2.2
1	D	132	GLY	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EPE	A	1003	15/15	0.87	0.15	57,59,62,62	0
4	EPE	B	2003	15/15	0.87	0.16	51,54,60,62	0
3	APR	A	1002	36/36	0.97	0.08	16,22,39,45	0
4	EPE	D	4003	15/15	0.98	0.09	19,23,27,27	0
3	APR	D	4002	36/36	0.98	0.08	16,23,25,26	0
3	APR	B	2002	36/36	0.98	0.08	15,19,42,43	0
3	APR	C	3002	36/36	0.98	0.08	16,19,23,23	0
4	EPE	C	3003	15/15	0.98	0.09	15,23,27,28	0
2	ZN	B	2001	1/1	0.99	0.07	22,22,22,22	0
2	ZN	A	1001	1/1	1.00	0.07	23,23,23,23	0
2	ZN	C	3001	1/1	1.00	0.08	19,19,19,19	0
2	ZN	D	4001	1/1	1.00	0.07	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.