



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 25, 2017 – 05:54 PM EST

PDB ID : 3PKI  
Title : Human SIRT6 crystal structure in complex with ADP ribose  
Authors : Pan, P.W.; Dong, A.; Qiu, W.; Loppnau, P.; Wang, J.; Ravichandran, M.;  
Bochkarev, A.; Bountra, C.; Weigelt, J.; Arrowsmith, C.H.; Min, J.; Edwards,  
A.M.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-11-11  
Resolution : 2.04 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/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:

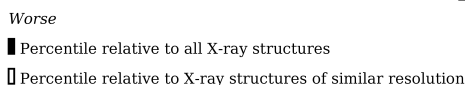
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442



**i**

## X-RAY DIFFRACTION

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	355	<div> <div>2%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
1	B	355	<div> <div>75%</div> <div>•</div> <div>22%</div> </div>
1	C	355	<div> <div>%</div> <div>75%</div> <div>•</div> <div>22%</div> </div>
1	D	355	<div> <div>%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
1	E	355	<div> <div>%</div> <div>73%</div> <div>5%</div> <div>22%</div> </div>
1	F	355	<div> <div>%</div> <div>73%</div> <div>•</div> <div>23%</div> </div>



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
5	SO4	B	360	-	-	-	X
5	SO4	C	364	-	-	-	X



## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14193 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	4	0
			2210	1388	407	404	11			
1	B	276	Total	C	N	O	S	0	3	0
			2158	1360	395	392	11			
1	C	277	Total	C	N	O	S	0	0	0
			2117	1336	385	385	11			
1	D	283	Total	C	N	O	S	0	3	0
			2143	1353	387	392	11			
1	E	276	Total	C	N	O	S	0	0	0
			2116	1338	381	386	11			
1	F	274	Total	C	N	O	S	0	6	0
			2147	1353	398	385	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
A	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
B	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
B	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
C	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
C	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
D	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
D	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
E	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
E	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
F	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
F	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total X 3 3	0	0
2	E	2	Total X 2 2	0	0
2	B	6	Total X 6 6	0	0
2	C	7	Total X 7 7	0	0
2	A	2	Total X 2 2	0	0
2	F	6	Total X 6 6	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

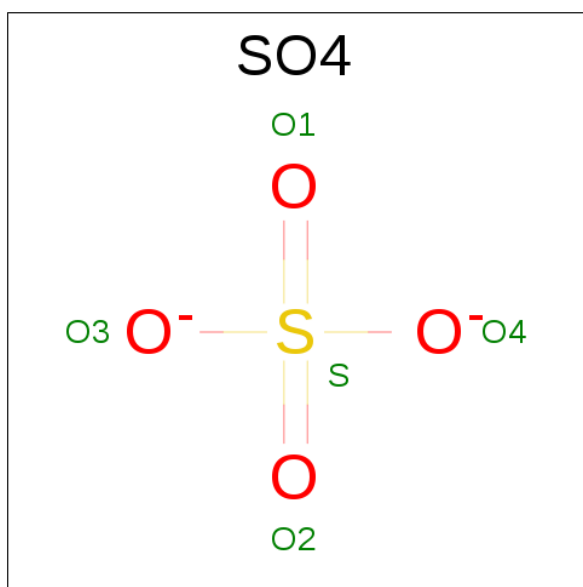
- Molecule 4 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).





- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





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

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

- Molecule 6 is water.

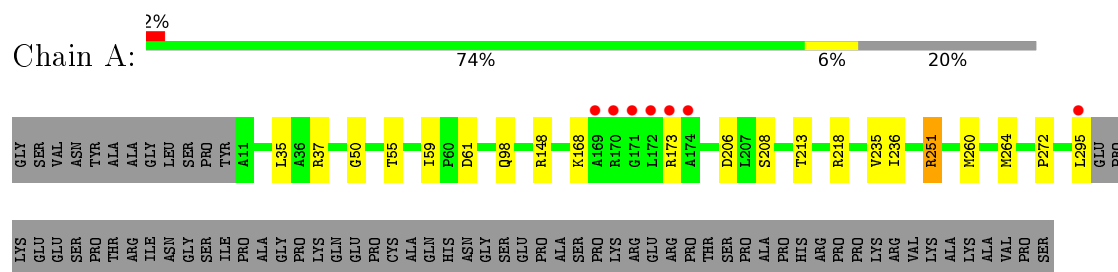
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	159	Total	O	0	0
			159	159		
6	B	162	Total	O	0	0
			162	162		
6	C	170	Total	O	0	0
			170	170		
6	D	170	Total	O	0	0
			170	170		
6	E	145	Total	O	0	0
			145	145		
6	F	133	Total	O	0	0
			133	133		



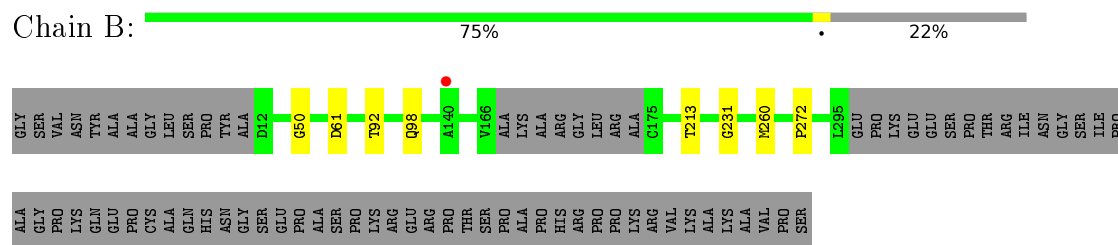
### 3 Residue-property plots [i](#)

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.

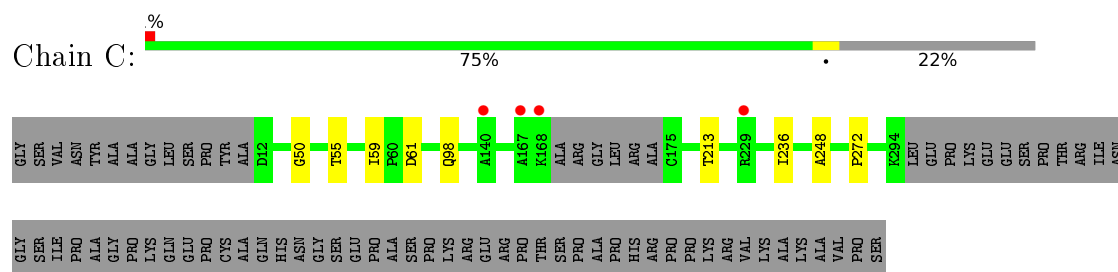
- Molecule 1: NAD-dependent deacetylase sirtuin-6



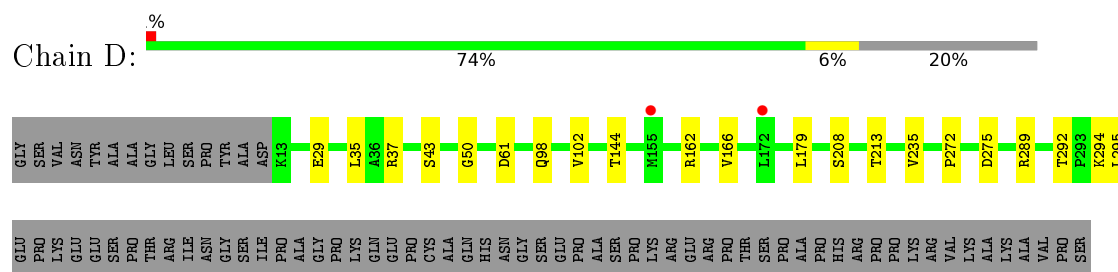
- Molecule 1: NAD-dependent deacetylase sirtuin-6



- Molecule 1: NAD-dependent deacetylase sirtuin-6

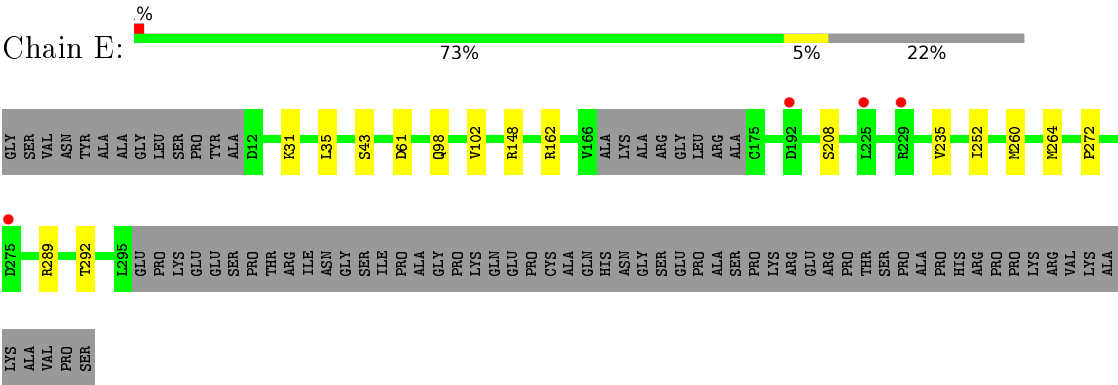


- Molecule 1: NAD-dependent deacetylase sirtuin-6

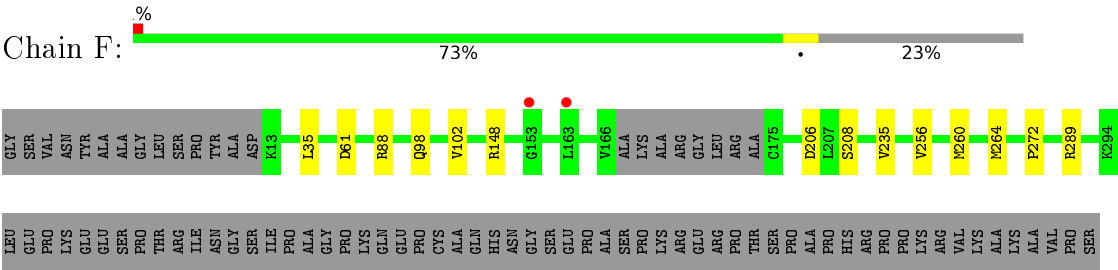




● Molecule 1: NAD-dependent deacetylase sirtuin-6



● Molecule 1: NAD-dependent deacetylase sirtuin-6





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.37Å 90.20Å 90.18Å 118.09° 91.39° 115.80°	Depositor
Resolution (Å)	29.87 – 2.04 45.68 – 2.04	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.87-2.04) 77.4 (45.68-2.04)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.183 , 0.213 0.187 , 0.223	Depositor DCC
$R_{free}$ test set	5784 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for h,-h-k,-l 0.012 for -h,-k-l,l 0.000 for -h,h+k+l,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, ZN, SO4, AR6

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	0.51	0/2258	0.56	0/3066
1	B	0.50	0/2208	0.55	0/2998
1	C	0.51	0/2164	0.55	0/2942
1	D	0.50	0/2191	0.57	0/2986
1	E	0.51	0/2163	0.56	0/2939
1	F	0.50	0/2194	0.56	0/2982
All	All	0.50	0/13178	0.56	0/17913

There are no bond length outliers.

There are no bond angle outliers.

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	2210	0	2196	10	0
1	B	2158	0	2154	5	0
1	C	2117	0	2096	5	0
1	D	2143	0	2098	12	0
1	E	2116	0	2096	9	0
1	F	2147	0	2126	7	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	0	0	0
2	C	7	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	36	0	21	1	0
4	B	36	0	21	1	0
4	C	36	0	21	1	0
4	D	36	0	21	1	0
4	E	36	0	21	1	0
4	F	36	0	21	2	0
5	A	25	0	0	0	0
5	B	15	0	0	0	0
5	C	20	0	0	0	0
5	D	15	0	0	1	0
5	E	30	0	0	0	0
5	F	10	0	0	0	0
6	A	159	0	0	0	0
6	B	162	0	0	0	0
6	C	170	0	0	0	0
6	D	170	0	0	0	0
6	E	145	0	0	0	0
6	F	133	0	0	0	0
All	All	14193	0	12892	44	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 2.

The worst 5 of 44 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:F:98:GLN:HB2	1:F:272:PRO:HD3	1.79	0.64
1:A:236:ILE:HB	1:A:251[B]:ARG:HD3	1.81	0.62
1:D:98:GLN:HB2	1:D:272:PRO:HD3	1.86	0.58
1:F:256[A]:VAL:HG23	4:F:2000:AR6:C2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:HG21	1:D:166:VAL:HG21	1.85	0.58

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	286/355 (81%)	280 (98%)	6 (2%)	0	100	100
1	B	275/355 (78%)	271 (98%)	4 (2%)	0	100	100
1	C	273/355 (77%)	270 (99%)	3 (1%)	0	100	100
1	D	284/355 (80%)	280 (99%)	4 (1%)	0	100	100
1	E	272/355 (77%)	268 (98%)	4 (2%)	0	100	100
1	F	276/355 (78%)	274 (99%)	2 (1%)	0	100	100
All	All	1666/2130 (78%)	1643 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	233/297 (78%)	227 (97%)	6 (3%)	54	47
1	B	231/297 (78%)	231 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	223/297 (75%)	223 (100%)	0	100	100
1	D	222/297 (75%)	218 (98%)	4 (2%)	66	62
1	E	223/297 (75%)	221 (99%)	2 (1%)	84	84
1	F	225/297 (76%)	222 (99%)	3 (1%)	76	74
All	All	1357/1782 (76%)	1342 (99%)	15 (1%)	82	79

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	29	GLU
1	D	43	SER
1	F	88	ARG
1	A	251[B]	ARG
1	E	208	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 61 ligands modelled in this entry, 26 are unknown and 6 are monoatomic - leaving 29 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
4	AR6	A	2000	-	34,39,39	0.90	1 (2%)	37,60,60	1.72	3 (8%)
5	SO4	A	356	-	4,4,4	0.18	0	6,6,6	0.20	0
5	SO4	A	357	-	4,4,4	0.32	0	6,6,6	0.12	0
5	SO4	A	358	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	A	359	-	4,4,4	0.97	0	6,6,6	0.16	0
5	SO4	A	360	-	4,4,4	0.27	0	6,6,6	0.09	0
4	AR6	B	2000	-	34,39,39	0.90	1 (2%)	37,60,60	1.74	3 (8%)
5	SO4	B	360	-	4,4,4	0.38	0	6,6,6	0.09	0
5	SO4	B	361	-	4,4,4	1.00	0	6,6,6	0.30	0
5	SO4	B	362	-	4,4,4	0.11	0	6,6,6	0.14	0
4	AR6	C	2000	-	34,39,39	0.89	1 (2%)	37,60,60	1.74	3 (8%)
5	SO4	C	361	-	4,4,4	0.87	0	6,6,6	0.21	0
5	SO4	C	362	-	4,4,4	0.27	0	6,6,6	0.27	0
5	SO4	C	363	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SO4	C	364	-	4,4,4	0.87	0	6,6,6	0.28	0
4	AR6	D	2000	-	34,39,39	0.92	1 (2%)	37,60,60	1.63	3 (8%)
5	SO4	D	357	-	4,4,4	0.19	0	6,6,6	0.19	0
5	SO4	D	358	-	4,4,4	0.10	0	6,6,6	0.06	0
5	SO4	D	359	-	4,4,4	0.19	0	6,6,6	0.07	0
4	AR6	E	2000	-	34,39,39	0.91	1 (2%)	37,60,60	1.63	3 (8%)
5	SO4	E	356	-	4,4,4	0.13	0	6,6,6	0.15	0
5	SO4	E	357	-	4,4,4	0.08	0	6,6,6	0.06	0
5	SO4	E	358	-	4,4,4	0.88	0	6,6,6	0.19	0
5	SO4	E	359	-	4,4,4	0.16	0	6,6,6	0.07	0
5	SO4	E	360	-	4,4,4	0.13	0	6,6,6	0.15	0
5	SO4	E	361	-	4,4,4	0.82	0	6,6,6	0.13	0
4	AR6	F	2000	-	34,39,39	0.92	1 (2%)	37,60,60	1.60	3 (8%)
5	SO4	F	360	-	4,4,4	1.05	0	6,6,6	0.45	0
5	SO4	F	361	-	4,4,4	0.51	0	6,6,6	0.14	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
4	AR6	A	2000	-	-	0/18/54/54	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	356	-	-	0/0/0/0	0/0/0/0
5	SO4	A	357	-	-	0/0/0/0	0/0/0/0
5	SO4	A	358	-	-	0/0/0/0	0/0/0/0
5	SO4	A	359	-	-	0/0/0/0	0/0/0/0
5	SO4	A	360	-	-	0/0/0/0	0/0/0/0
4	AR6	B	2000	-	-	0/18/54/54	0/4/4/4
5	SO4	B	360	-	-	0/0/0/0	0/0/0/0
5	SO4	B	361	-	-	0/0/0/0	0/0/0/0
5	SO4	B	362	-	-	0/0/0/0	0/0/0/0
4	AR6	C	2000	-	-	0/18/54/54	0/4/4/4
5	SO4	C	361	-	-	0/0/0/0	0/0/0/0
5	SO4	C	362	-	-	0/0/0/0	0/0/0/0
5	SO4	C	363	-	-	0/0/0/0	0/0/0/0
5	SO4	C	364	-	-	0/0/0/0	0/0/0/0
4	AR6	D	2000	-	-	0/18/54/54	0/4/4/4
5	SO4	D	357	-	-	0/0/0/0	0/0/0/0
5	SO4	D	358	-	-	0/0/0/0	0/0/0/0
5	SO4	D	359	-	-	0/0/0/0	0/0/0/0
4	AR6	E	2000	-	-	0/18/54/54	0/4/4/4
5	SO4	E	356	-	-	0/0/0/0	0/0/0/0
5	SO4	E	357	-	-	0/0/0/0	0/0/0/0
5	SO4	E	358	-	-	0/0/0/0	0/0/0/0
5	SO4	E	359	-	-	0/0/0/0	0/0/0/0
5	SO4	E	360	-	-	0/0/0/0	0/0/0/0
5	SO4	E	361	-	-	0/0/0/0	0/0/0/0
4	AR6	F	2000	-	-	0/18/54/54	0/4/4/4
5	SO4	F	360	-	-	0/0/0/0	0/0/0/0
5	SO4	F	361	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2000	AR6	C5-C4	2.87	1.47	1.40
4	C	2000	AR6	C5-C4	2.98	1.47	1.40
4	F	2000	AR6	C5-C4	3.00	1.47	1.40
4	E	2000	AR6	C5-C4	3.05	1.47	1.40
4	B	2000	AR6	C5-C4	3.10	1.47	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2000	AR6	N3-C2-N1	-8.11	122.50	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2000	AR6	N3-C2-N1	-8.00	122.58	128.87
4	D	2000	AR6	N3-C2-N1	-7.83	122.72	128.87
4	A	2000	AR6	N3-C2-N1	-7.67	122.85	128.87
4	E	2000	AR6	N3-C2-N1	-7.63	122.88	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2000	AR6	1	0
4	B	2000	AR6	1	0
4	C	2000	AR6	1	0
4	D	2000	AR6	1	0
5	D	357	SO4	1	0
4	E	2000	AR6	1	0
4	F	2000	AR6	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	285/355 (80%)	-0.16	7 (2%) 61 67	15, 29, 51, 73	0
1	B	276/355 (77%)	-0.35	1 (0%) 93 94	15, 28, 47, 68	0
1	C	277/355 (78%)	-0.27	4 (1%) 78 82	16, 29, 47, 83	0
1	D	283/355 (79%)	-0.25	2 (0%) 89 91	18, 31, 51, 67	0
1	E	276/355 (77%)	-0.17	4 (1%) 78 82	19, 32, 51, 68	0
1	F	274/355 (77%)	-0.18	2 (0%) 89 91	19, 34, 56, 67	0
All	All	1671/2130 (78%)	-0.23	20 (1%) 81 84	15, 31, 51, 83	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	167	ALA	4.4
1	A	170	ARG	4.1
1	A	171	GLY	3.8
1	A	174	ALA	3.4
1	A	172	LEU	3.4

### 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 ⓘ

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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	B	360	5/5	0.96	0.20	5.61	54,58,59,59	0
5	SO4	C	364	5/5	0.97	0.15	3.97	40,45,46,46	0
5	SO4	B	361	5/5	0.97	0.15	1.86	44,48,50,50	0
5	SO4	C	362	5/5	0.96	0.20	1.66	57,61,62,62	0
5	SO4	A	356	5/5	0.96	0.15	1.49	57,62,62,62	0
5	SO4	E	360	5/5	0.92	0.20	1.39	67,72,73,73	0
5	SO4	A	359	5/5	0.99	0.12	1.18	41,46,47,47	0
5	SO4	F	361	5/5	0.91	0.18	1.04	78,82,83,84	0
5	SO4	A	358	5/5	0.95	0.13	0.97	64,68,69,70	0
5	SO4	A	360	5/5	0.90	0.17	0.72	91,95,96,96	0
5	SO4	E	358	5/5	0.97	0.12	0.48	46,50,52,52	0
5	SO4	F	360	5/5	0.98	0.13	-0.08	53,58,59,59	0
5	SO4	D	359	5/5	0.91	0.16	-0.15	91,95,96,96	0
4	AR6	B	2000	36/36	0.98	0.09	-0.17	17,22,33,45	0
5	SO4	E	356	5/5	0.97	0.10	-0.23	52,57,57,58	0
4	AR6	E	2000	36/36	0.98	0.09	-0.55	17,27,37,42	0
5	SO4	A	357	5/5	0.97	0.11	-0.56	62,66,67,67	0
4	AR6	D	2000	36/36	0.98	0.08	-0.62	20,26,39,41	0
4	AR6	F	2000	36/36	0.97	0.08	-0.71	22,29,39,55	0
5	SO4	D	357	5/5	0.98	0.09	-0.73	44,48,49,50	0
4	AR6	C	2000	36/36	0.98	0.08	-0.77	14,21,27,31	0
5	SO4	B	362	5/5	0.97	0.09	-0.77	53,57,58,58	0
5	SO4	C	361	5/5	0.97	0.11	-1.01	42,47,48,48	0
4	AR6	A	2000	36/36	0.98	0.08	-1.12	14,23,30,37	0
3	ZN	D	1000	1/1	0.99	0.07	-1.41	41,41,41,41	0
3	ZN	A	1000	1/1	0.99	0.06	-1.56	34,34,34,34	0
3	ZN	E	1000	1/1	0.98	0.07	-2.22	37,37,37,37	0
3	ZN	C	1000	1/1	0.97	0.06	-2.59	42,42,42,42	0
3	ZN	F	1000	1/1	0.98	0.06	-2.91	51,51,51,51	0
3	ZN	B	1000	1/1	0.99	0.03	-3.71	42,42,42,42	0
2	UNX	B	355	1/1	0.92	0.39	-	43,43,43,43	0
2	UNX	A	355	1/1	0.82	0.39	-	36,36,36,36	0
2	UNX	C	360	1/1	0.81	0.25	-	37,37,37,37	0
2	UNX	E	355	1/1	0.78	0.35	-	43,43,43,43	0
5	SO4	E	361	5/5	0.89	0.30	-	100,105,105,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UNX	C	355	1/1	0.69	0.23	-	49,49,49,49	0
2	UNX	C	359	1/1	0.88	0.40	-	46,46,46,46	0
2	UNX	C	357	1/1	0.72	0.35	-	50,50,50,50	0
2	UNX	C	356	1/1	0.89	0.32	-	46,46,46,46	0
5	SO4	C	363	5/5	0.90	0.22	-	80,84,85,86	0
2	UNX	B	357	1/1	0.92	0.30	-	45,45,45,45	0
2	UNX	B	358	1/1	0.68	0.30	-	45,45,45,45	0
2	UNX	C	358	1/1	0.80	0.28	-	53,53,53,53	0
2	UNX	B	359	1/1	0.73	0.15	-	49,49,49,49	0
2	UNX	D	356	1/1	0.82	0.17	-	30,30,30,30	0
2	UNX	F	356	1/1	0.86	0.33	-	42,42,42,42	0
5	SO4	D	358	5/5	0.97	0.11	-	72,76,77,78	0
2	UNX	F	355	1/1	0.86	0.28	-	53,53,53,53	0
2	UNX	F	357	1/1	0.73	0.27	-	51,51,51,51	0
2	UNX	B	354	1/1	0.92	0.45	-	39,39,39,39	0
5	SO4	E	357	5/5	0.94	0.12	-	86,91,91,92	0
2	UNX	F	354	1/1	0.89	0.42	-	53,53,53,53	0
2	UNX	F	359	1/1	0.73	0.33	-	30,30,30,30	0
2	UNX	F	358	1/1	0.89	0.32	-	54,54,54,54	0
5	SO4	E	359	5/5	0.94	0.15	-	70,74,76,76	0
2	UNX	D	355	1/1	0.67	0.39	-	47,47,47,47	0
2	UNX	D	354	1/1	0.93	0.32	-	50,50,50,50	0
2	UNX	E	354	1/1	0.81	0.42	-	48,48,48,48	0
2	UNX	C	354	1/1	0.88	0.18	-	45,45,45,45	0
2	UNX	B	356	1/1	0.67	0.34	-	39,39,39,39	0
2	UNX	A	354	1/1	0.64	0.35	-	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.