



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:32 AM GMT

PDB ID : 2DEW  
Title : Crystal structure of human peptidylarginine deiminase 4 in complex with histone H3 N-terminal tail including Arg8  
Authors : Arita, K.; Shimizu, T.; Hashimoto, H.; Hidaka, Y.; Yamada, M.; Sato, M.  
Deposited on : 2006-02-18  
Resolution : 2.10 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

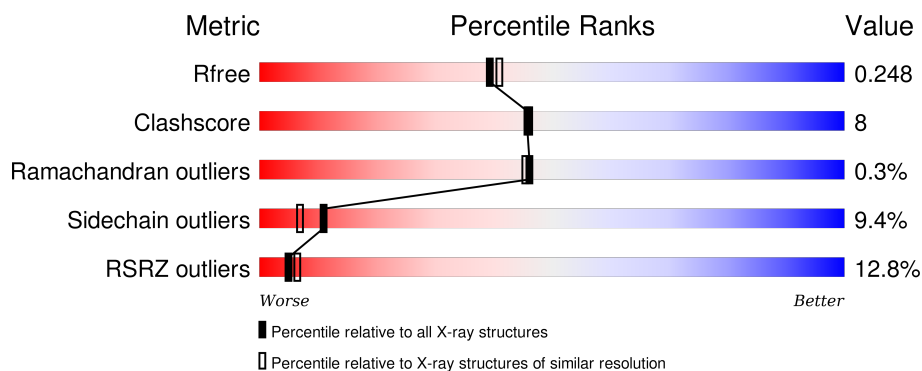
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	X	671	
2	A	10	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5234 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 deiminase type IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	629	Total	C	N	O	S	0	0	0
			4952	3161	831	925	35			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-7	GLY	-	CLONING ARTIFACT	UNP Q9UM07
X	-6	PRO	-	CLONING ARTIFACT	UNP Q9UM07
X	-5	LEU	-	CLONING ARTIFACT	UNP Q9UM07
X	-4	GLY	-	CLONING ARTIFACT	UNP Q9UM07
X	-3	SER	-	CLONING ARTIFACT	UNP Q9UM07
X	-2	PRO	-	CLONING ARTIFACT	UNP Q9UM07
X	-1	GLU	-	CLONING ARTIFACT	UNP Q9UM07
X	0	PHE	-	CLONING ARTIFACT	UNP Q9UM07
X	645	ALA	CYS	ENGINEERED	UNP Q9UM07

- Molecule 2 is a protein called 10-mer peptide from histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	5	Total	C	N	O	0	0	0
			38	22	9	7			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	5	Total	Ca	0	0
			5	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		

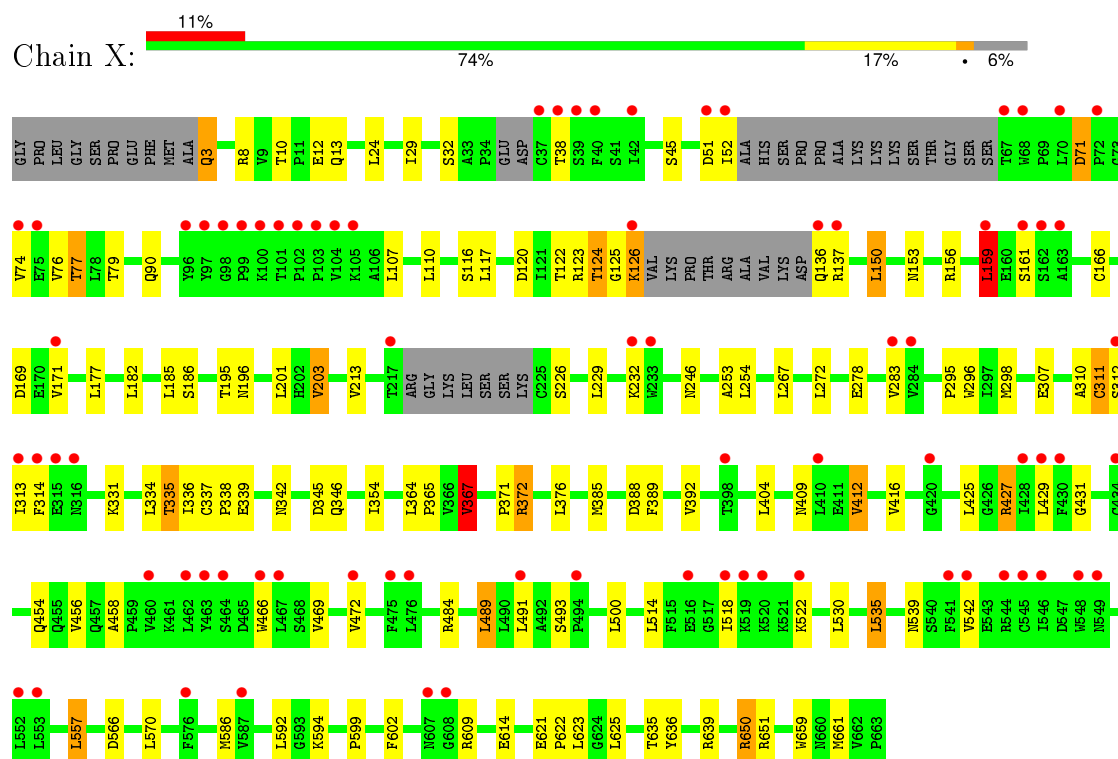
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	X	222	Total	O	0	0
			222	222		

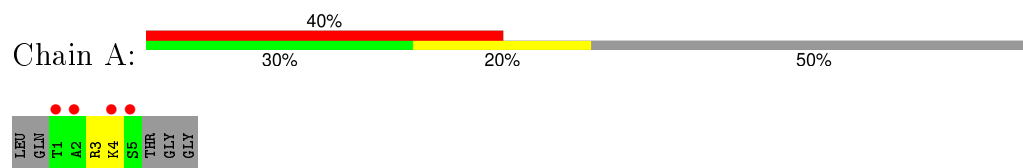
### 3 Residue-property plots

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 deiminase type IV



- Molecule 2: 10-mer peptide from histone H3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.27Å 60.77Å 115.15Å 90.00° 124.26° 90.00°	Depositor
Resolution (Å)	38.34 – 2.10 38.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (38.34-2.10) 97.9 (38.34-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.202 , 0.241 0.209 , 0.248	Depositor DCC
$R_{free}$ test set	4878 reflections (11.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48004 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, SO4

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	X	0.57	2/5071 (0.0%)	0.74	6/6881 (0.1%)
2	A	0.82	0/37	0.90	0/47
All	All	0.58	2/5108 (0.0%)	0.74	6/6928 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	311	CYS	CB-SG	-5.94	1.72	1.81
1	X	203	VAL	CB-CG1	-5.01	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	427	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	X	367	VAL	CB-CA-C	-6.42	99.21	111.40
1	X	412	VAL	CB-CA-C	-6.21	99.60	111.40
1	X	159	LEU	CA-CB-CG	6.06	129.23	115.30
1	X	372	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	X	372	ARG	NE-CZ-NH2	-5.05	117.78	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	X	4952	0	4913	77	0
2	A	38	0	45	1	0
3	X	5	0	0	0	0
4	X	15	0	0	0	0
5	A	2	0	0	0	0
5	X	222	0	0	4	1
All	All	5234	0	4958	77	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 8.

All (77) 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:X:651:ARG:NH1	5:X:1096:HOH:O	2.05	0.89
1:X:416:VAL:HG21	1:X:557:LEU:O	1.78	0.84
1:X:313:ILE:HB	1:X:338:PRO:HA	1.63	0.80
1:X:120:ASP:HB2	1:X:126:LYS:HD3	1.64	0.78
1:X:650:ARG:HH11	1:X:650:ARG:HG3	1.55	0.71
1:X:203:VAL:HG12	1:X:267:LEU:HD23	1.80	0.64
1:X:310:ALA:O	1:X:336:ILE:HA	1.97	0.64
1:X:354:ILE:HD13	1:X:367:VAL:HG13	1.79	0.64
1:X:296:TRP:H	1:X:454:GLN:HE21	1.47	0.62
1:X:416:VAL:CG2	1:X:557:LEU:O	2.46	0.62
1:X:307:GLU:OE2	1:X:335:THR:CG2	2.48	0.61
1:X:195:THR:HG22	1:X:196:ASN:ND2	2.18	0.59
1:X:313:ILE:CB	1:X:338:PRO:HA	2.32	0.59
1:X:409:ASN:HD22	1:X:472:VAL:H	1.51	0.59
1:X:307:GLU:OE2	1:X:335:THR:HG21	2.05	0.57
1:X:586:MET:HA	1:X:599:PRO:HG2	1.86	0.57
1:X:203:VAL:CG1	1:X:267:LEU:CD2	2.84	0.56
1:X:123:ARG:HD3	1:X:659:TRP:CD1	2.41	0.55
1:X:334:LEU:HD11	1:X:336:ILE:CD1	2.36	0.55
1:X:466:TRP:CZ3	1:X:542:VAL:HG13	2.42	0.54
1:X:311:CYS:SG	1:X:311:CYS:O	2.66	0.53
1:X:10:THR:HG22	1:X:32:SER:CB	2.38	0.53
1:X:153:ASN:HB3	1:X:166:CYS:HB3	1.91	0.53
1:X:296:TRP:H	1:X:454:GLN:NE2	2.06	0.53
1:X:409:ASN:HD21	1:X:431:GLY:HA3	1.74	0.52
1:X:51:ASP:HB2	1:X:77:THR:HG23	1.90	0.52
1:X:365:PRO:HD2	1:X:388:ASP:O	2.10	0.51
1:X:52:ILE:HD12	1:X:76:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:334:LEU:C	1:X:334:LEU:HD13	2.30	0.51
1:X:45:SER:OG	1:X:90:GLN:NE2	2.44	0.51
1:X:232:LYS:O	1:X:232:LYS:HD3	2.11	0.50
1:X:650:ARG:CG	1:X:650:ARG:HH11	2.22	0.50
1:X:311:CYS:CB	1:X:337:CYS:HB3	2.42	0.50
1:X:425:LEU:HD12	1:X:456:VAL:HG22	1.94	0.50
1:X:213:VAL:HG13	1:X:229:LEU:HB2	1.93	0.49
1:X:311:CYS:HB2	1:X:342:ASN:OD1	2.13	0.49
1:X:203:VAL:HG12	1:X:267:LEU:CD2	2.43	0.49
1:X:29:ILE:CD1	1:X:76:VAL:HG21	2.43	0.48
1:X:313:ILE:HG12	1:X:336:ILE:CG2	2.43	0.48
1:X:635:THR:HG23	1:X:636:TYR:HD1	1.77	0.48
1:X:124:THR:OG1	1:X:125:GLY:N	2.45	0.48
1:X:416:VAL:HG23	5:X:1107:HOH:O	2.14	0.48
1:X:166:CYS:HB2	1:X:254:LEU:HD22	1.95	0.48
1:X:518:ILE:HD11	1:X:602:PHE:CD1	2.48	0.48
1:X:71:ASP:C	1:X:71:ASP:OD1	2.51	0.48
1:X:226:SER:HB2	5:X:1025:HOH:O	2.13	0.48
1:X:29:ILE:HD12	1:X:76:VAL:HG21	1.96	0.47
1:X:150:LEU:HD13	1:X:253:ALA:HB2	1.97	0.47
1:X:518:ILE:HD11	1:X:602:PHE:CG	2.49	0.46
1:X:311:CYS:HB3	1:X:337:CYS:HB3	1.98	0.46
1:X:345:ASP:OD2	1:X:372:ARG:NH2	2.50	0.45
1:X:623:LEU:HB2	1:X:625:LEU:CD2	2.46	0.45
1:X:296:TRP:N	1:X:454:GLN:HE21	2.11	0.45
1:X:10:THR:HG22	1:X:32:SER:HB2	1.99	0.45
1:X:456:VAL:HG23	1:X:661:MET:SD	2.56	0.44
1:X:650:ARG:HD3	5:X:1100:HOH:O	2.17	0.44
1:X:469:VAL:HG11	2:A:3:ARG:HD3	1.98	0.44
1:X:535:LEU:HD22	1:X:539:ASN:ND2	2.33	0.44
1:X:295:PRO:HA	1:X:454:GLN:NE2	2.34	0.43
1:X:74:VAL:O	1:X:74:VAL:HG13	2.18	0.43
1:X:156:ARG:HD2	1:X:161:SER:O	2.19	0.43
1:X:171:VAL:HG11	1:X:177:LEU:HD21	2.01	0.43
1:X:3:GLN:HE21	1:X:24:LEU:H	1.67	0.43
1:X:126:LYS:HE3	1:X:182:LEU:HB3	2.01	0.42
1:X:354:ILE:CD1	1:X:367:VAL:HG13	2.48	0.42
1:X:489:LEU:HD13	1:X:491:LEU:HG	2.01	0.42
1:X:122:THR:OG1	1:X:124:THR:HG23	2.20	0.42
1:X:296:TRP:CZ3	1:X:298:MET:HG3	2.54	0.41
1:X:186:SER:OG	1:X:246:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:493:SER:CB	1:X:566:ASP:HB3	2.50	0.41
1:X:621:GLU:N	1:X:622:PRO:CD	2.83	0.41
1:X:456:VAL:CG2	1:X:661:MET:SD	3.09	0.41
1:X:71:ASP:O	1:X:74:VAL:HG12	2.20	0.41
1:X:339:GLU:HA	1:X:342:ASN:HB2	2.03	0.41
1:X:272:LEU:CD2	1:X:283:VAL:HG22	2.51	0.40
1:X:371:PRO:O	1:X:372:ARG:C	2.60	0.40
1:X:296:TRP:CH2	1:X:298:MET:CG	3.05	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:X:931:HOH:O	5:X:993:HOH:O[2_555]	2.17	0.03

## 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	X	619/671 (92%)	587 (95%)	30 (5%)	2 (0%)	46	45
2	A	3/10 (30%)	3 (100%)	0	0	100	100
All	All	622/681 (91%)	590 (95%)	30 (5%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	159	LEU
1	X	458	ALA

### 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	X	559/593 (94%)	507 (91%)	52 (9%)	11	7
2	A	4/7 (57%)	3 (75%)	1 (25%)	1	0
All	All	563/600 (94%)	510 (91%)	53 (9%)	11	7

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	3	GLN
1	X	8	ARG
1	X	12	GLU
1	X	13	GLN
1	X	38	THR
1	X	71	ASP
1	X	77	THR
1	X	79	THR
1	X	107	LEU
1	X	110	LEU
1	X	116	SER
1	X	117	LEU
1	X	124	THR
1	X	126	LYS
1	X	136	GLN
1	X	137	ARG
1	X	150	LEU
1	X	159	LEU
1	X	169	ASP
1	X	185	LEU
1	X	201	LEU
1	X	278	GLU
1	X	312	SER
1	X	314	PHE
1	X	331	LYS
1	X	335	THR
1	X	346	GLN

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Mol	Chain	Res	Type
1	X	364	LEU
1	X	367	VAL
1	X	376	LEU
1	X	385	MET
1	X	389	PHE
1	X	392	VAL
1	X	404	LEU
1	X	412	VAL
1	X	427	ARG
1	X	429	LEU
1	X	484	ARG
1	X	489	LEU
1	X	500	LEU
1	X	514	LEU
1	X	522	LYS
1	X	530	LEU
1	X	535	LEU
1	X	557	LEU
1	X	570	LEU
1	X	592	LEU
1	X	594	LYS
1	X	609	ARG
1	X	614	GLU
1	X	639	ARG
1	X	650	ARG
2	A	4	LYS

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

Mol	Chain	Res	Type
1	X	3	GLN
1	X	13	GLN
1	X	90	GLN
1	X	178	GLN
1	X	196	ASN
1	X	246	ASN
1	X	276	ASN
1	X	409	ASN
1	X	438	ASN
1	X	448	GLN
1	X	454	GLN
1	X	505	GLN

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Mol	Chain	Res	Type
1	X	538	HIS

### 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 [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	SO4	X	905	-	4,4,4	0.25	0	6,6,6	0.23	0
4	SO4	X	906	-	4,4,4	0.24	0	6,6,6	0.16	0
4	SO4	X	907	-	4,4,4	0.13	0	6,6,6	0.15	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	SO4	X	905	-	-	0/0/0/0	0/0/0/0
4	SO4	X	906	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	X	907	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	X	629/671 (93%)	0.68	77 (12%) <b>5</b> <b>7</b>	40, 50, 67, 80	0
2	A	5/10 (50%)	2.42	4 (80%) <b>0</b> <b>0</b>	58, 61, 70, 71	0
All	All	634/681 (93%)	0.69	81 (12%) <b>5</b> <b>6</b>	40, 50, 67, 80	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	312	SER	6.7
1	X	98	GLY	6.6
1	X	74	VAL	5.5
1	X	68	TRP	5.5
1	X	519	LYS	5.3
1	X	38	THR	5.3
1	X	462	LEU	5.2
1	X	159	LEU	5.0
1	X	546	ILE	4.9
1	X	70	LEU	4.8
2	A	2	ALA	4.5
1	X	37	CYS	4.5
1	X	103	PRO	4.4
1	X	520	LYS	4.3
1	X	40	PHE	4.0
1	X	314	PHE	3.9
1	X	476	LEU	3.8
1	X	104	VAL	3.7
1	X	545	CYS	3.7
1	X	475	PHE	3.6
1	X	217	THR	3.6
1	X	587	VAL	3.5
1	X	99	PRO	3.5
1	X	466	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	548	TRP	3.4
1	X	608	GLY	3.4
1	X	542	VAL	3.4
1	X	97	TYR	3.3
1	X	283	VAL	3.3
1	X	233	TRP	3.3
2	A	1	THR	3.2
1	X	75	GLU	3.2
1	X	52	ILE	3.2
1	X	472	VAL	3.2
1	X	316	ASN	3.0
1	X	460	VAL	3.0
1	X	51	ASP	3.0
1	X	126	LYS	2.9
1	X	102	PRO	2.9
1	X	491	LEU	2.9
1	X	552	LEU	2.9
1	X	232	LYS	2.9
1	X	96	TYR	2.9
1	X	522	LYS	2.8
1	X	463	TYR	2.8
2	A	4	LYS	2.8
1	X	467	LEU	2.8
1	X	430	PHE	2.7
1	X	518	ILE	2.7
1	X	100	LYS	2.7
1	X	161	SER	2.7
1	X	315	GLU	2.7
1	X	434	CYS	2.6
1	X	171	VAL	2.6
1	X	162	SER	2.5
1	X	553	LEU	2.5
1	X	284	VAL	2.5
1	X	137	ARG	2.5
1	X	105	LYS	2.5
1	X	544	ARG	2.4
1	X	39	SER	2.4
1	X	464	SER	2.4
1	X	101	THR	2.4
1	X	429	LEU	2.4
1	X	136	GLN	2.3
1	X	541	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	576	PHE	2.2
1	X	42	ILE	2.2
1	X	313	ILE	2.2
1	X	67	THR	2.2
1	X	516	GLU	2.2
1	X	398	THR	2.2
1	X	428	ILE	2.2
1	X	72	PRO	2.1
1	X	549	ASN	2.1
1	X	607	ASN	2.1
1	X	420	GLY	2.0
1	X	163	ALA	2.0
1	X	410	LEU	2.0
1	X	494	PRO	2.0
2	A	5	SER	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<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
4	SO4	X	906	5/5	0.95	0.20	1.77	86,87,87,87	0
3	CA	X	904	1/1	0.97	0.14	-0.25	44,44,44,44	0
4	SO4	X	905	5/5	0.97	0.14	-0.36	90,90,91,91	0
3	CA	X	902	1/1	0.97	0.10	-0.73	53,53,53,53	0
3	CA	X	901	1/1	0.98	0.11	-0.84	47,47,47,47	0
3	CA	X	903	1/1	0.97	0.08	-1.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	X	900	1/1	0.99	0.05	-3.39	40,40,40,40	0
4	SO4	X	907	5/5	0.94	0.21	-	75,75,75,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.