



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 05:07 pm GMT

PDB ID : 1BS8  
Title : PEPTIDE DEFORMYLASE AS ZN<sup>2+</sup> CONTAINING FORM IN COMPLEX WITH TRIPEPTIDE MET-ALA-SER  
Authors : Becker, A.; Schlichting, I.; Kabsch, W.; Groche, D.; Schultz, S.; Wagner, A.F.V.  
Deposited on : 1998-09-01  
Resolution : 2.20 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

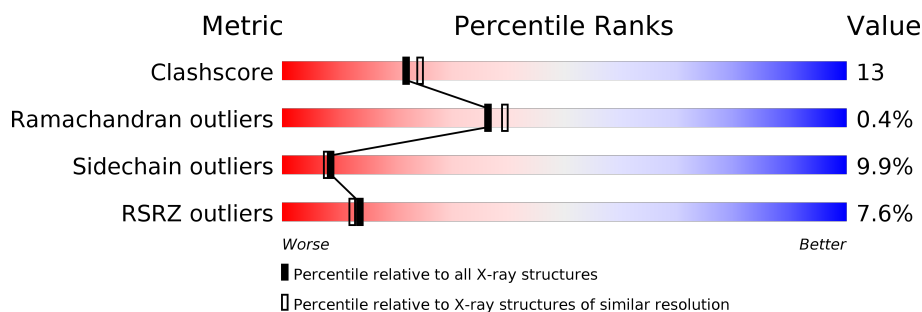
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	168	<div> <div>10%</div> <div>65%</div> <div>30%</div> <div>• •</div> </div>
1	B	168	<div> <div>5%</div> <div>69%</div> <div>29%</div> <div>•</div> </div>
1	C	168	<div> <div>7%</div> <div>71%</div> <div>24%</div> <div>5%</div> </div>
2	D	3	<div> <div>33%</div> <div>67%</div> <div>33%</div> </div>
2	E	3	<div> <div>33%</div> <div>67%</div> </div>
2	F	3	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4345 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 (PEPTIDE DEFORMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	9	0
			1383	863	247	267	6			
1	B	168	Total	C	N	O	S	0	1	0
			1350	846	241	257	6			
1	C	168	Total	C	N	O	S	0	7	0
			1374	858	242	268	6			

- Molecule 2 is a protein called PROTEIN (MET-ALA-SER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	S	0	0	0
			20	11	3	5	1			
2	E	3	Total	C	N	O	S	0	0	0
			20	11	3	5	1			
2	F	3	Total	C	N	O	S	0	0	0
			20	11	3	5	1			

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

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

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



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

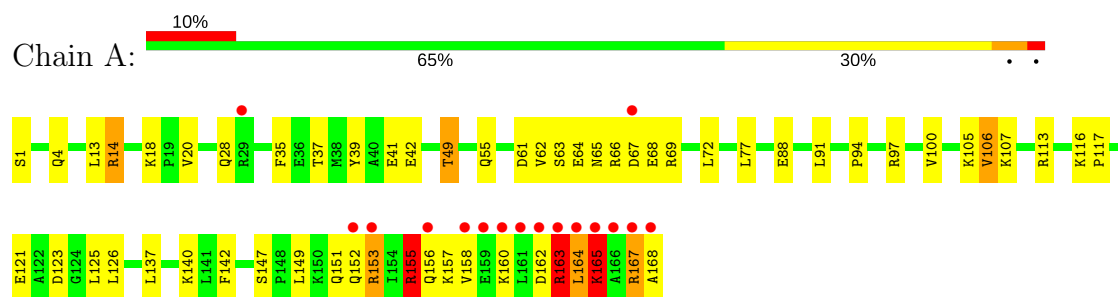
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		
5	B	62	Total	O	0	0
			62	62		
5	C	62	Total	O	0	0
			62	62		
5	E	1	Total	O	0	0
			1	1		

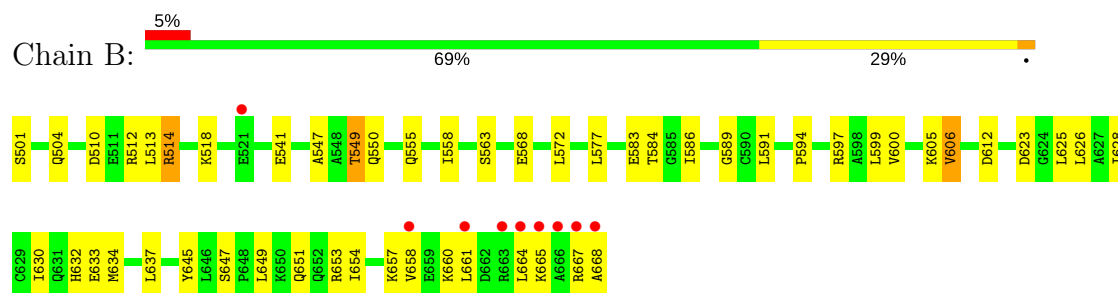
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

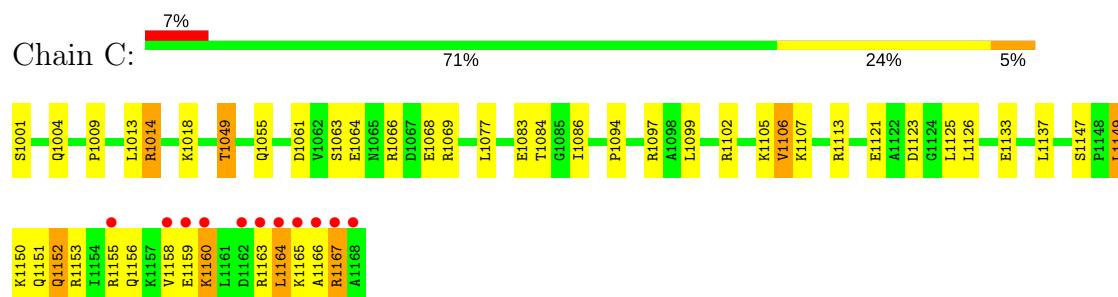
#### • Molecule 1: PROTEIN (PEPTIDE DEFORMYLASE)



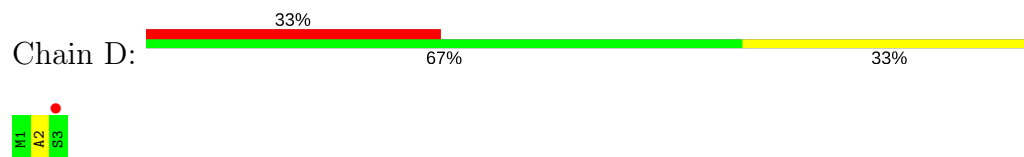
#### • Molecule 1: PROTEIN (PEPTIDE DEFORMYLASE)



#### • Molecule 1: PROTEIN (PEPTIDE DEFORMYLASE)



#### • Molecule 2: PROTEIN (MET-ALA-SER)



- Molecule 2: PROTEIN (MET-ALA-SER)

Chain E:  33% 33% 67%



- Molecule 2: PROTEIN (MET-ALA-SER)

Chain F:  33% 33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.10Å 64.20Å 84.70Å 90.00° 123.30° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 9.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (6.00-2.20) 92.4 (9.99-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.261 0.209 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 90.3	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.033 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4345	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 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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: ZN, 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	A	0.52	0/1369	0.66	0/1849
1	B	0.52	0/1362	0.63	0/1832
1	C	0.55	0/1368	0.66	0/1844
2	D	0.88	0/19	0.70	0/22
2	E	0.73	0/19	0.61	0/22
2	F	0.86	0/19	1.03	0/22
All	All	0.54	0/4156	0.65	0/5591

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	A	0	5
1	B	0	2
1	C	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	155	ARG	Sidechain
1	A	156	GLN	Mainchain
1	A	163	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	165	LYS	Peptide
1	B	514	ARG	Sidechain
1	B	583	GLU	Mainchain
1	C	1014	ARG	Sidechain

## 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	1383	0	1427	44	0
1	B	1350	0	1392	27	0
1	C	1374	0	1406	37	0
2	D	20	0	21	1	0
2	E	20	0	21	4	0
2	F	20	0	21	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	10	0	0	0	0
5	A	40	0	0	2	0
5	B	62	0	0	1	0
5	C	62	0	0	2	0
5	E	1	0	0	0	0
All	All	4345	0	4288	108	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 13.

All (108) 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:A:160:LYS:O	1:A:163:ARG:HB3	1.71	0.90
1:A:66:ARG:HH11	1:A:66:ARG:HG3	1.32	0.90
1:B:541[1]:GLU:HG3	1:B:591:LEU:HD22	1.70	0.73
1:A:162:ASP:HA	1:A:165:LYS:HB2	1.71	0.72
1:A:39:TYR:CZ	1:A:66:ARG:HG2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:O	1:A:151:GLN:HG3	1.95	0.67
1:A:164:LEU:N	1:A:164:LEU:HD13	2.10	0.67
1:B:577:LEU:HD11	1:B:606:VAL:HG22	1.78	0.65
1:A:77:LEU:HD11	1:A:106:VAL:HG22	1.78	0.65
1:C:1165:LYS:N	1:C:1167:ARG:HH12	1.94	0.64
1:A:163:ARG:HB3	1:A:164:LEU:HD13	1.80	0.64
1:A:35:PHE:CZ	1:A:69:ARG:HB3	2.32	0.64
1:B:661:LEU:O	1:B:665:LYS:HG2	1.97	0.64
1:C:1009:PRO:HG3	1:C:1155:ARG:HH21	1.62	0.64
1:A:63:SER:HB3	1:A:68:GLU:HB2	1.78	0.64
1:C:1147:SER:O	1:C:1151:GLN:HG3	1.98	0.64
1:A:153:ARG:HE	1:A:153:ARG:HA	1.63	0.62
1:A:153:ARG:O	1:A:157:LYS:HG3	1.99	0.62
1:C:1009:PRO:HG3	1:C:1155:ARG:NH2	2.15	0.62
1:A:116[1]:LYS:HG2	1:A:117:PRO:HD2	1.81	0.61
1:C:1149:LEU:O	1:C:1153:ARG:HG3	2.00	0.61
1:B:667:ARG:HD2	1:B:668:ALA:H	1.64	0.61
1:C:1152:GLN:O	1:C:1156:GLN:HG3	2.01	0.60
1:C:1077:LEU:HD11	1:C:1106:VAL:HG22	1.83	0.59
1:C:1086:ILE:O	1:C:1099:LEU:HA	2.03	0.59
1:B:586:ILE:HG12	1:B:628:ILE:HD13	1.83	0.59
1:C:1165:LYS:N	1:C:1167:ARG:NH1	2.52	0.57
1:A:153:ARG:HA	1:A:153:ARG:NE	2.20	0.57
1:C:1069:ARG:HD2	5:C:52:HOH:O	2.04	0.56
1:B:647:SER:O	1:B:651:GLN:HG3	2.05	0.56
1:B:589:GLY:O	2:E:1:MET:HB3	2.06	0.56
1:A:116[1]:LYS:HE2	1:A:117:PRO:O	2.06	0.55
1:A:66:ARG:NH1	1:A:66:ARG:HG3	2.08	0.55
1:B:600:VAL:HG22	1:B:645:TYR:HB2	1.87	0.55
1:C:1166:ALA:N	1:C:1167:ARG:NH1	2.55	0.54
1:C:1152:GLN:HG3	1:C:1156:GLN:HE21	1.72	0.53
1:B:518:LYS:O	1:B:555:GLN:HA	2.08	0.53
1:A:164:LEU:N	1:A:164:LEU:CD1	2.71	0.53
1:C:1150:LYS:NZ	1:C:1153:ARG:HH21	2.07	0.53
1:C:1160:LYS:HG2	1:C:1164:LEU:HD23	1.91	0.53
1:C:1009:PRO:HB3	1:C:1155:ARG:NE	2.23	0.53
1:C:1155:ARG:NH2	1:C:1159:GLU:OE2	2.42	0.53
1:C:1049:THR:HB	5:C:37:HOH:O	2.09	0.53
1:C:1150:LYS:HZ2	1:C:1153:ARG:HH21	1.56	0.52
1:A:37:THR:O	1:A:41:GLU:HG2	2.10	0.51
1:B:577:LEU:CD1	1:B:606:VAL:HG22	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1159:GLU:O	1:C:1163:ARG:HB2	2.12	0.50
1:A:77:LEU:CD1	1:A:106:VAL:HG22	2.42	0.49
1:C:1163:ARG:C	1:C:1165:LYS:H	2.16	0.49
1:C:1009:PRO:HB3	1:C:1155:ARG:CZ	2.42	0.49
1:C:1094:PRO:HG2	1:C:1158:VAL:HG13	1.94	0.49
1:A:91:LEU:HD12	1:A:91:LEU:N	2.28	0.48
1:B:667:ARG:HD2	1:B:668:ALA:N	2.28	0.48
1:B:586:ILE:O	1:B:599:LEU:HA	2.12	0.48
1:A:164:LEU:HD13	1:A:164:LEU:H	1.78	0.48
1:B:605:LYS:HG2	1:B:623:ASP:HB3	1.95	0.48
1:B:558:ILE:HB	1:B:572:LEU:HB2	1.95	0.48
1:C:1133:GLU:OE2	2:F:1:MET:N	2.47	0.48
1:A:18:LYS:O	1:A:55:GLN:HA	2.14	0.47
1:A:94:PRO:HG2	1:A:158:VAL:HG13	1.96	0.47
1:C:1097:ARG:NH2	2:F:3:SER:OG	2.47	0.47
1:B:632:HIS:CG	2:E:1:MET:HG2	2.49	0.47
1:C:1018:LYS:O	1:C:1055:GLN:HA	2.15	0.47
1:C:1049:THR:HG21	1:C:1137:LEU:HA	1.97	0.47
1:C:1077:LEU:CD1	1:C:1106:VAL:HG22	2.45	0.47
1:B:661:LEU:HG	1:B:665:LYS:HE3	1.96	0.46
1:A:41:GLU:O	1:A:42[1]:GLU:HB2	2.16	0.46
1:C:1061:ASP:HB3	1:C:1066:ARG:HH21	1.80	0.46
1:C:1063:SER:HB3	1:C:1068:GLU:HB2	1.97	0.46
1:B:653:ARG:O	1:B:657:LYS:HG3	2.16	0.45
1:C:1107:LYS:HD2	1:C:1121[1]:GLU:CG	2.47	0.45
1:B:654:ILE:O	1:B:658:VAL:HG23	2.16	0.45
1:B:594:PRO:HG2	1:B:658:VAL:HG13	1.97	0.45
1:B:549:THR:HG21	1:B:637:LEU:HA	1.99	0.45
1:A:28:GLN:HB3	1:A:113[1]:ARG:NH2	2.32	0.45
1:B:563:SER:HB3	1:B:568:GLU:HB2	1.99	0.45
1:A:167:ARG:HE	1:A:168:ALA:C	2.21	0.44
1:A:160:LYS:O	1:A:164:LEU:HD13	2.18	0.44
1:A:49:THR:HB	5:A:2004:HOH:O	2.18	0.44
1:B:612:ASP:HB2	5:B:110:HOH:O	2.19	0.43
1:A:162:ASP:C	1:A:165:LYS:H	2.21	0.43
1:C:1105:LYS:HG2	1:C:1123:ASP:HB3	2.01	0.43
1:C:1164:LEU:C	1:C:1167:ARG:HH12	2.21	0.43
1:C:1149:LEU:HD12	1:C:1149:LEU:HA	1.78	0.42
1:A:100:VAL:HG21	1:A:142:PHE:HB2	2.01	0.42
1:A:149:LEU:HD22	1:A:152[2]:GLN:HE22	1.84	0.42
1:A:140:LYS:HE3	5:A:2012:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HG22	1:A:55:GLN:OE1	2.20	0.42
1:B:633:GLU:OE2	2:E:1:MET:N	2.49	0.41
1:B:510:ASP:OD2	1:B:512:ARG:NH2	2.50	0.41
1:B:547:ALA:O	1:B:550:GLN:HB2	2.20	0.41
1:A:107:LYS:HD2	1:A:121:GLU:HG2	2.01	0.41
1:C:1163:ARG:O	1:C:1165:LYS:N	2.48	0.41
1:B:597:ARG:NH2	2:E:3:SER:O	2.53	0.41
1:A:63:SER:CB	1:A:68:GLU:HB2	2.49	0.41
1:A:35:PHE:CE1	1:A:69:ARG:HG2	2.55	0.41
1:C:1083:GLU:HA	1:C:1102:ARG:O	2.21	0.41
1:C:1150:LYS:NZ	1:C:1153:ARG:NH2	2.69	0.41
1:A:88:GLU:O	1:A:97:ARG:HA	2.20	0.41
1:B:630:ILE:O	1:B:634:MET:HG3	2.21	0.41
1:A:105:LYS:HG2	1:A:123:ASP:HB3	2.03	0.40
1:A:61:ASP:HB2	1:A:69:ARG:HA	2.03	0.40
1:A:49:THR:HG21	1:A:137:LEU:HA	2.04	0.40
1:A:39:TYR:CE1	1:A:66:ARG:HG2	2.56	0.40
1:A:97:ARG:NH1	2:D:2:ALA:O	2.55	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	175/168 (104%)	165 (94%)	9 (5%)	1 (1%)	27	28
1	B	167/168 (99%)	164 (98%)	3 (2%)	0	100	100
1	C	173/168 (103%)	164 (95%)	8 (5%)	1 (1%)	27	28
2	D	1/3 (33%)	1 (100%)	0	0	100	100
2	E	1/3 (33%)	1 (100%)	0	0	100	100
2	F	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	518/513 (101%)	496 (96%)	20 (4%)	2 (0%)	36	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1164	LEU
1	A	163	ARG

### 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	139/148 (94%)	122 (88%)	17 (12%)	5	4
1	B	147/148 (99%)	135 (92%)	12 (8%)	12	12
1	C	141/148 (95%)	127 (90%)	14 (10%)	8	8
2	D	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
All	All	433/450 (96%)	390 (90%)	43 (10%)	8	8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	4	GLN
1	A	13	LEU
1	A	14	ARG
1	A	49	THR
1	A	62	VAL
1	A	64	GLU
1	A	67	ASP
1	A	72	LEU
1	A	106	VAL

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Mol	Chain	Res	Type
1	A	125	LEU
1	A	126	LEU
1	A	153	ARG
1	A	155	ARG
1	A	164	LEU
1	A	165	LYS
1	A	167	ARG
1	B	501	SER
1	B	504	GLN
1	B	513	LEU
1	B	514	ARG
1	B	549	THR
1	B	584	THR
1	B	606	VAL
1	B	625	LEU
1	B	626	LEU
1	B	649	LEU
1	B	660	LYS
1	B	664	LEU
1	C	1001	SER
1	C	1004	GLN
1	C	1013	LEU
1	C	1014	ARG
1	C	1049	THR
1	C	1084	THR
1	C	1106	VAL
1	C	1113	ARG
1	C	1125	LEU
1	C	1126	LEU
1	C	1149	LEU
1	C	1152	GLN
1	C	1160	LYS
1	C	1167	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	652	GLN
1	C	1004	GLN
1	C	1152	GLN
1	C	1156	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	B	3001	-	4,4,4	0.35	0	6,6,6	0.37	0
4	SO4	B	3002	-	4,4,4	0.42	0	6,6,6	0.25	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	B	3001	-	-	0/0/0/0	0/0/0/0
4	SO4	B	3002	-	-	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	A	168/168 (100%)	0.24	16 (9%) 8 7	16, 31, 60, 77	0
1	B	168/168 (100%)	-0.26	9 (5%) 26 24	15, 27, 58, 70	0
1	C	168/168 (100%)	-0.15	11 (6%) 19 18	15, 27, 61, 77	0
2	D	3/3 (100%)	1.43	1 (33%) 0 0	39, 39, 49, 57	0
2	E	3/3 (100%)	1.74	1 (33%) 0 0	56, 56, 57, 58	0
2	F	3/3 (100%)	1.04	1 (33%) 0 0	41, 41, 48, 55	0
All	All	513/513 (100%)	-0.03	39 (7%) 14 12	15, 29, 62, 77	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	ALA	15.9
1	C	1166	ALA	10.1
1	A	165	LYS	8.6
1	B	668	ALA	8.5
1	A	166	ALA	8.4
1	C	1168	ALA	7.0
1	B	666	ALA	6.6
1	C	1167	ARG	6.4
1	C	1164	LEU	6.2
1	A	163	ARG	6.1
1	A	162	ASP	6.0
1	A	167	ARG	5.9
1	B	658	VAL	4.6
1	C	1165	LYS	4.3
1	A	164	LEU	4.2
1	B	667	ARG	4.1
2	E	3	SER	3.7
1	A	29	ARG	3.6
1	A	161	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	665	LYS	3.1
1	C	1159	GLU	3.0
1	C	1163	ARG	3.0
1	A	160	LYS	3.0
1	A	159	GLU	2.9
1	A	153	ARG	2.9
1	B	663	ARG	2.9
1	C	1155	ARG	2.7
2	F	3	SER	2.5
1	C	1162	ASP	2.5
1	A	67	ASP	2.5
1	B	661	LEU	2.4
1	B	664	LEU	2.4
1	C	1160	LYS	2.4
1	A	152[1]	GLN	2.4
1	C	1158	VAL	2.4
2	D	3	SER	2.4
1	A	158	VAL	2.2
1	A	156	GLN	2.2
1	B	521	GLU	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	SO4	B	3001	5/5	0.97	0.17	48,48,50,51	0
4	SO4	B	3002	5/5	0.97	0.18	46,48,48,48	0
3	ZN	A	2001	1/1	0.99	0.02	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	C	2001	1/1	1.00	0.01	24,24,24,24	0
3	ZN	B	2001	1/1	1.00	0.03	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.