



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:38 PM GMT

PDB ID : 1BS7  
Title : PEPTIDE DEFORMYLASE AS NI2+ CONTAINING FORM  
Authors : Becker, A.; Schlichting, I.; Kabsch, W.; Groche, D.; Schultz, S.; Wagner, A.F.V.  
Deposited on : 1998-09-01  
Resolution : 2.50 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

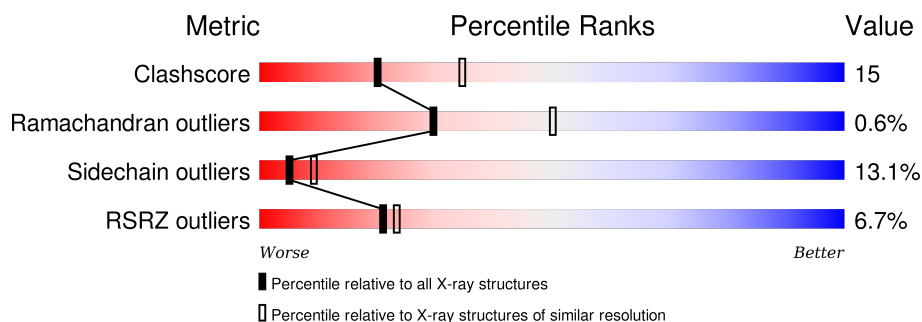
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	
1	B	168	
1	C	168	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4182 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	0	0
			1346	844	241	255	6			
1	B	168	Total	C	N	O	S	0	0	0
			1346	844	241	255	6			
1	C	168	Total	C	N	O	S	0	0	0
			1346	844	241	255	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

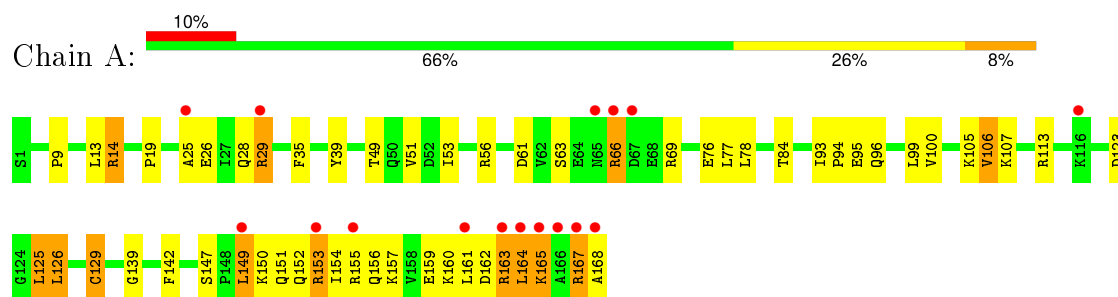
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	48	Total 48	O 48	0	0
4	C	50	Total 50	O 50	0	0

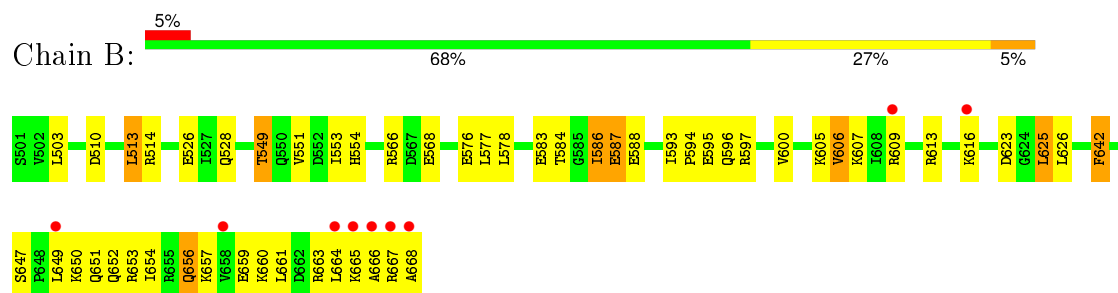
### 3 Residue-property plots [i](#)

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

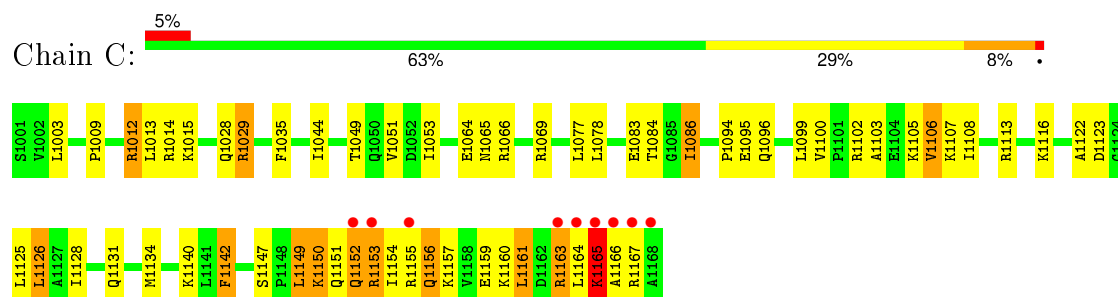
#### • Molecule 1: PROTEIN (PEPTIDE DEFORMYLASE)



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.40 Å   64.00 Å   84.50 Å 90.00°   123.00°   90.00°	Depositor
Resolution (Å)	6.00 – 2.50 9.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (6.00-2.50) 95.3 (9.98-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.203   ,   0.272 0.205   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40   ,   86.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 21555 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.61	0/1361	0.70	0/1830
1	B	0.61	0/1361	0.65	0/1830
1	C	0.61	0/1361	0.69	1/1830 (0.1%)
All	All	0.61	0/4083	0.68	1/5490 (0.0%)

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	2
1	B	0	2
1	C	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1161	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	ARG	Sidechain
1	A	163	ARG	Mainchain
1	B	554	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	B	583	GLU	Mainchain
1	C	1083	GLU	Mainchain

## 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	1346	0	1393	40	0
1	B	1346	0	1390	32	0
1	C	1346	0	1390	53	0
2	B	10	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
4	A	33	0	0	1	0
4	B	48	0	0	1	0
4	C	50	0	0	2	0
All	All	4182	0	4173	121	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 15.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:ALA:H	1:C:1131:GLN:HE22	1.21	0.89
1:A:77:LEU:HD11	1:A:106:VAL:HG22	1.57	0.87
1:B:577:LEU:HD11	1:B:606:VAL:HG22	1.56	0.84
1:A:19:PRO:HG2	1:C:1066:ARG:HG2	1.63	0.81
1:B:653:ARG:O	1:B:657:LYS:HG3	1.80	0.80
1:C:1077:LEU:HD11	1:C:1106:VAL:HG22	1.63	0.80
1:C:1167:ARG:HG2	1:C:1167:ARG:HH11	1.48	0.79
1:C:1149:LEU:HD22	1:C:1153:ARG:HH21	1.48	0.79
1:C:1149:LEU:HD22	1:C:1153:ARG:NH2	1.99	0.78
1:C:1167:ARG:NE	1:C:1167:ARG:HA	2.02	0.75
1:A:162:ASP:HA	1:A:165:LYS:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:VAL:HG23	1:B:553:ILE:HD12	1.74	0.69
1:B:586:ILE:HD12	1:B:587:GLU:H	1.58	0.69
1:A:51:VAL:HG23	1:A:53:ILE:HD12	1.76	0.68
1:C:1086:ILE:HD13	1:C:1128:ILE:HD13	1.75	0.67
1:C:1051:VAL:HG23	1:C:1053:ILE:HD12	1.77	0.66
1:A:164:LEU:N	1:A:164:LEU:HD13	2.11	0.66
1:C:1166:ALA:H	1:C:1167:ARG:HH12	1.43	0.66
1:C:1166:ALA:H	1:C:1167:ARG:NH1	1.93	0.65
1:A:25:ALA:O	1:A:29:ARG:HG2	1.98	0.64
1:C:1150:LYS:HA	1:C:1153:ARG:HD2	1.80	0.64
1:A:77:LEU:CD1	1:A:106:VAL:HG22	2.28	0.62
1:C:1164:LEU:O	1:C:1165:LYS:HG2	1.99	0.62
1:A:26:GLU:HG3	4:A:2033:HOH:O	1.99	0.62
1:C:1159:GLU:HB3	1:C:1163:ARG:HH21	1.66	0.61
1:C:1100:VAL:HG21	1:C:1142:PHE:HB2	1.81	0.61
1:A:100:VAL:HG21	1:A:142:PHE:HB2	1.84	0.60
1:A:164:LEU:O	1:A:167:ARG:HB2	2.01	0.60
1:A:25:ALA:HB1	1:A:29:ARG:NH1	2.17	0.60
1:C:1161:LEU:O	1:C:1165:LYS:HB2	2.01	0.60
1:B:577:LEU:CD1	1:B:606:VAL:HG22	2.31	0.59
1:C:1086:ILE:HD13	1:C:1128:ILE:CD1	2.31	0.59
1:B:659:GLU:HB3	1:B:663:ARG:HH21	1.69	0.58
1:C:1077:LEU:CD1	1:C:1106:VAL:HG22	2.33	0.57
1:C:1165:LYS:H	1:C:1167:ARG:HH12	1.51	0.57
1:C:1163:ARG:HB3	1:C:1164:LEU:HD22	1.87	0.56
1:A:159:GLU:HB3	1:A:163:ARG:HH21	1.69	0.56
1:B:578:LEU:HD12	1:B:607:LYS:HD3	1.88	0.56
1:C:1103:ALA:N	1:C:1131:GLN:HE22	1.99	0.55
1:B:652:GLN:O	1:B:656:GLN:HG2	2.06	0.55
1:A:78:LEU:HD12	1:A:107:LYS:HD3	1.88	0.55
1:C:1012:ARG:HG3	1:C:1015:LYS:HD2	1.89	0.55
1:A:147:SER:O	1:A:151:GLN:HG3	2.07	0.55
1:A:167:ARG:HD3	1:A:168:ALA:N	2.23	0.54
1:A:19:PRO:HG3	1:C:1065:ASN:HA	1.88	0.54
1:C:1009:PRO:HG3	1:C:1155:ARG:HE	1.73	0.54
1:A:14:ARG:NH2	1:A:139:GLY:O	2.41	0.54
1:C:1078:LEU:HD12	1:C:1107:LYS:HD3	1.89	0.54
1:A:25:ALA:HB1	1:A:29:ARG:HH11	1.73	0.53
1:B:526:GLU:OE2	1:C:1029:ARG:HD2	2.09	0.53
1:B:663:ARG:HB3	1:B:664:LEU:HD13	1.92	0.52
1:A:125:LEU:O	1:A:129:CYS:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:LEU:HD23	1:C:1003:LEU:HD23	1.92	0.51
1:B:663:ARG:HB3	1:B:664:LEU:CD1	2.41	0.51
1:A:61:ASP:OD2	1:A:66:ARG:HA	2.10	0.51
1:C:1153:ARG:O	1:C:1157:LYS:HG3	2.10	0.51
1:B:605:LYS:HG2	1:B:623:ASP:HB3	1.94	0.50
1:B:647:SER:O	1:B:651:GLN:HG3	2.11	0.50
1:C:1167:ARG:NE	1:C:1167:ARG:CA	2.73	0.49
1:A:56:ARG:HH11	1:A:56:ARG:HG2	1.78	0.49
1:B:593:ILE:HG22	1:B:596:GLN:HB2	1.93	0.49
1:A:9:PRO:HG3	1:A:155:ARG:HE	1.76	0.49
1:C:1105:LYS:HG2	1:C:1123:ASP:HB3	1.95	0.49
1:B:578:LEU:HB2	1:B:607:LYS:HD2	1.94	0.49
1:A:105:LYS:HG2	1:A:123:ASP:HB3	1.94	0.49
1:C:1108:ILE:HG21	1:C:1134:MET:HE1	1.95	0.48
1:B:642:PHE:C	1:B:642:PHE:CD1	2.87	0.48
1:C:1147:SER:O	1:C:1151:GLN:HG3	2.12	0.48
1:C:1096:GLN:HG3	1:C:1154:ILE:HG23	1.96	0.48
1:A:161:LEU:HA	1:A:164:LEU:HD22	1.96	0.48
1:A:78:LEU:HB2	1:A:107:LYS:HD2	1.96	0.47
1:B:596:GLN:HG3	1:B:654:ILE:HG23	1.96	0.47
1:A:164:LEU:N	1:A:164:LEU:CD1	2.76	0.47
1:C:1149:LEU:HD22	1:C:1153:ARG:CZ	2.44	0.47
1:C:1035:PHE:CE1	1:C:1069:ARG:HG2	2.50	0.47
1:A:39:TYR:CE1	1:A:66:ARG:HG3	2.50	0.47
1:C:1163:ARG:O	1:C:1165:LYS:N	2.48	0.46
1:A:28:GLN:HB3	1:A:113:ARG:NH2	2.30	0.46
1:C:1069:ARG:HD2	4:C:47:HOH:O	2.15	0.46
1:C:1166:ALA:N	1:C:1167:ARG:NH1	2.64	0.46
1:B:594:PRO:O	1:B:595:GLU:HB2	2.16	0.46
1:A:142:PHE:C	1:A:142:PHE:CD1	2.89	0.45
1:B:600:VAL:HG21	1:B:642:PHE:HB2	1.97	0.45
1:B:605:LYS:HB3	1:B:605:LYS:HE3	1.84	0.45
1:C:1078:LEU:HB2	1:C:1107:LYS:HD2	1.98	0.45
1:A:126:LEU:HA	1:A:126:LEU:HD23	1.85	0.45
1:C:1095:GLU:OE2	1:C:1161:LEU:HD11	2.17	0.45
1:C:1152:GLN:O	1:C:1156:GLN:HG2	2.17	0.45
1:B:510:ASP:O	1:B:513:LEU:HB2	2.17	0.44
1:B:549:THR:HB	4:B:15:HOH:O	2.17	0.44
1:C:1142:PHE:C	1:C:1142:PHE:CD1	2.91	0.44
1:A:94:PRO:O	1:A:95:GLU:HB2	2.17	0.44
1:A:39:TYR:CE1	1:A:66:ARG:NE	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:ILE:HG22	1:C:1066:ARG:HH12	1.82	0.44
1:B:551:VAL:CG2	1:B:553:ILE:HD12	2.46	0.43
1:C:1164:LEU:HD22	1:C:1164:LEU:N	2.34	0.43
1:C:1094:PRO:O	1:C:1095:GLU:HB2	2.18	0.43
1:C:1167:ARG:HG2	1:C:1167:ARG:NH1	2.26	0.42
1:B:666:ALA:O	1:B:668:ALA:N	2.52	0.42
1:A:149:LEU:O	1:A:153:ARG:HG3	2.20	0.42
1:A:96:GLN:HG3	1:A:154:ILE:HG23	2.01	0.42
1:B:576:GLU:HG2	1:B:609:ARG:HB3	2.01	0.42
1:C:1102:ARG:HG3	1:C:1128:ILE:HG23	2.02	0.42
1:A:93:ILE:HG22	1:A:96:GLN:HB2	2.02	0.42
1:C:1095:GLU:HG3	4:C:105:HOH:O	2.19	0.42
1:A:35:PHE:CE1	1:A:69:ARG:HG2	2.55	0.41
1:C:1099:LEU:HD23	1:C:1099:LEU:C	2.40	0.41
1:B:588:GLU:O	1:B:597:ARG:HA	2.20	0.41
1:C:1044:ILE:HG22	1:C:1066:ARG:NH1	2.35	0.41
1:A:96:GLN:OE1	1:A:157:LYS:HD3	2.21	0.41
1:A:167:ARG:HE	1:A:168:ALA:C	2.24	0.41
1:A:63:SER:O	1:A:66:ARG:NH1	2.49	0.41
1:B:659:GLU:HB3	1:B:663:ARG:NH2	2.34	0.41
1:B:586:ILE:HA	1:B:586:ILE:HD13	1.82	0.41
1:B:528:GLN:HB3	1:B:613:ARG:NH2	2.36	0.41
1:B:625:LEU:HA	1:B:625:LEU:HD23	1.88	0.41
1:C:1096:GLN:OE1	1:C:1157:LYS:HD3	2.21	0.41
1:C:1028:GLN:HB3	1:C:1113:ARG:NH2	2.36	0.40
1:C:1122:ALA:HB1	1:C:1126:LEU:HB3	2.03	0.40
1:B:661:LEU:HB3	1:B:665:LYS:HE3	2.03	0.40
1:A:9:PRO:HG3	1:A:155:ARG:NE	2.37	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	166/168 (99%)	156 (94%)	9 (5%)	1 (1%)	30	50
1	B	166/168 (99%)	158 (95%)	8 (5%)	0	100	100
1	C	166/168 (99%)	155 (93%)	9 (5%)	2 (1%)	16	29
All	All	498/504 (99%)	469 (94%)	26 (5%)	3 (1%)	30	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1165	LYS
1	A	165	LYS
1	C	1163	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	148/148 (100%)	129 (87%)	19 (13%)	5	10
1	B	148/148 (100%)	130 (88%)	18 (12%)	6	11
1	C	148/148 (100%)	127 (86%)	21 (14%)	4	7
All	All	444/444 (100%)	386 (87%)	58 (13%)	5	9

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	ARG
1	A	29	ARG
1	A	49	THR
1	A	66	ARG
1	A	76	GLU
1	A	84	THR
1	A	99	LEU
1	A	106	VAL
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	126	LEU
1	A	129	CYS
1	A	149	LEU
1	A	150	LYS
1	A	152	GLN
1	A	156	GLN
1	A	160	LYS
1	A	164	LEU
1	A	167	ARG
1	B	513	LEU
1	B	514	ARG
1	B	549	THR
1	B	566	ARG
1	B	568	GLU
1	B	584	THR
1	B	586	ILE
1	B	587	GLU
1	B	606	VAL
1	B	616	LYS
1	B	625	LEU
1	B	626	LEU
1	B	642	PHE
1	B	649	LEU
1	B	650	LYS
1	B	656	GLN
1	B	660	LYS
1	B	667	ARG
1	C	1012	ARG
1	C	1013	LEU
1	C	1014	ARG
1	C	1029	ARG
1	C	1049	THR
1	C	1064	GLU
1	C	1084	THR
1	C	1086	ILE
1	C	1106	VAL
1	C	1116	LYS
1	C	1125	LEU
1	C	1126	LEU
1	C	1140	LYS
1	C	1142	PHE
1	C	1149	LEU

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Mol	Chain	Res	Type
1	C	1150	LYS
1	C	1152	GLN
1	C	1153	ARG
1	C	1156	GLN
1	C	1160	LYS
1	C	1165	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	652	GLN
1	C	1131	GLN

### 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 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	$\# Z  > 2$
2	SO4	B	3001	-	4,4,4	0.41	0	6,6,6	0.40	0
2	SO4	B	3002	-	4,4,4	0.54	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	3001	-	-	0/0/0/0	0/0/0/0
2	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 [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	A	168/168 (100%)	0.26	16 (9%) 10 11	20, 36, 66, 96	0
1	B	168/168 (100%)	-0.13	9 (5%) 29 33	19, 33, 62, 84	0
1	C	168/168 (100%)	-0.10	9 (5%) 29 33	17, 33, 65, 94	0
All	All	504/504 (100%)	0.01	34 (6%) 21 23	17, 34, 66, 96	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	668	ALA	10.7
1	A	168	ALA	9.0
1	C	1167	ARG	7.9
1	C	1168	ALA	7.8
1	C	1166	ALA	7.3
1	A	166	ALA	7.2
1	C	1164	LEU	6.7
1	A	165	LYS	5.7
1	A	163	ARG	5.5
1	B	667	ARG	5.4
1	B	666	ALA	5.1
1	C	1165	LYS	4.7
1	C	1155	ARG	4.5
1	A	161	LEU	4.4
1	A	164	LEU	4.4
1	A	167	ARG	4.3
1	A	29	ARG	4.3
1	B	665	LYS	3.9
1	A	155	ARG	3.2
1	B	658	VAL	3.1
1	C	1152	GLN	3.0
1	A	25	ALA	2.9
1	A	67	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1163	ARG	2.7
1	A	65	ASN	2.6
1	B	664	LEU	2.6
1	A	116	LYS	2.6
1	C	1153	ARG	2.5
1	A	66	ARG	2.4
1	A	153	ARG	2.4
1	A	149	LEU	2.4
1	B	649	LEU	2.3
1	B	609	ARG	2.1
1	B	616	LYS	2.1

## 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
3	NI	A	2001	1/1	0.98	0.03	-1.91	47,47,47,47	0
3	NI	B	2001	1/1	0.99	0.05	-2.32	32,32,32,32	0
3	NI	C	2001	1/1	0.99	0.04	-3.45	37,37,37,37	0
2	SO4	B	3001	5/5	0.94	0.23	-	50,53,54,59	0
2	SO4	B	3002	5/5	0.95	0.13	-	47,48,52,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.