



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 PM GMT

PDB ID : 4Q3B  
Title : PylD cocrystallized with L-Lysine-Ne-D-lysine and NAD+  
Authors : Quitterer, F.; Beck, P.; Bacher, A.; Groll, M.  
Deposited on : 2014-04-11  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

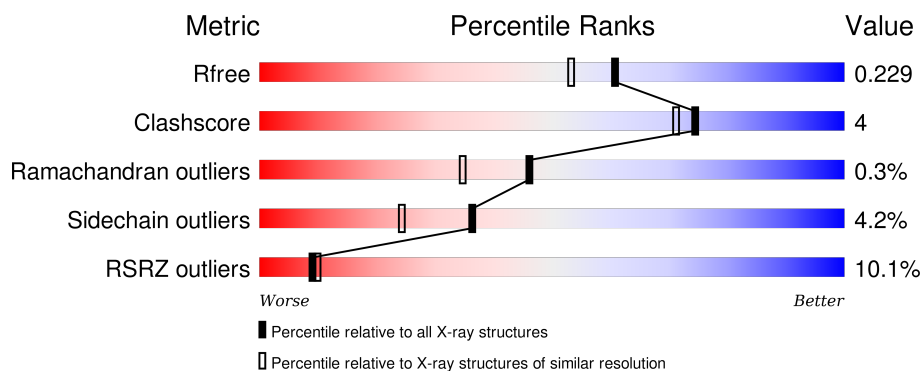
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	<div> <div>5%</div> <div>92%</div> <div>8%</div> </div>
1	B	260	<div> <div>4%</div> <div>91%</div> <div>8%</div> </div>
1	C	260	<div> <div>16%</div> <div>91%</div> <div>9%</div> </div>
1	D	260	<div> <div>15%</div> <div>90%</div> <div>10%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	902	-	-	-	X
3	NA	B	902	-	-	-	X
3	NA	C	902	-	-	-	X
4	MG	D	903	-	-	-	X
6	EDO	A	905	-	-	-	X
6	EDO	B	905	-	-	-	X
6	EDO	B	907	-	-	-	X
7	GOL	A	906	-	-	-	X
7	GOL	A	910	-	-	-	X
7	GOL	A	911	-	-	-	X
7	GOL	A	912	-	-	-	X
7	GOL	B	908	-	-	-	X
7	GOL	B	909	-	-	X	X
7	GOL	B	910	-	-	-	X
8	PEG	B	915	-	-	-	X
8	PEG	B	916	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8587 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.

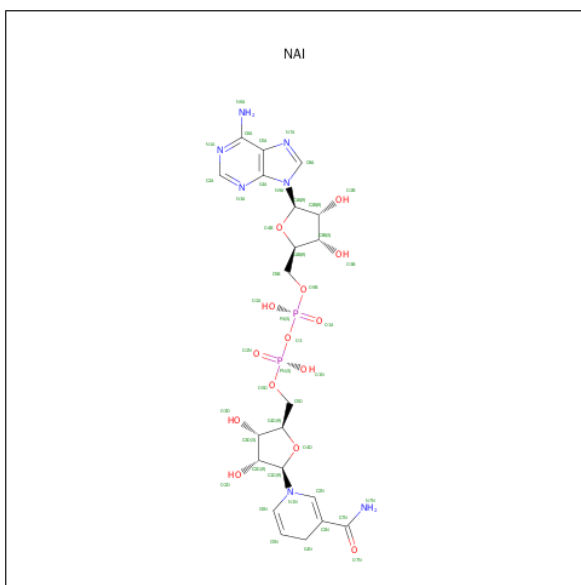
- Molecule 1 is a protein called PYLD, pyrrolysine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1962	1249	315	387	11			
1	B	260	Total	C	N	O	S	0	0	0
			1962	1249	315	387	11			
1	C	260	Total	C	N	O	S	0	0	0
			1962	1249	315	387	11			
1	D	260	Total	C	N	O	S	0	0	0
			1962	1249	315	387	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q46E80
B	0	SER	-	EXPRESSION TAG	UNP Q46E80
C	0	SER	-	EXPRESSION TAG	UNP Q46E80
D	0	SER	-	EXPRESSION TAG	UNP Q46E80

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

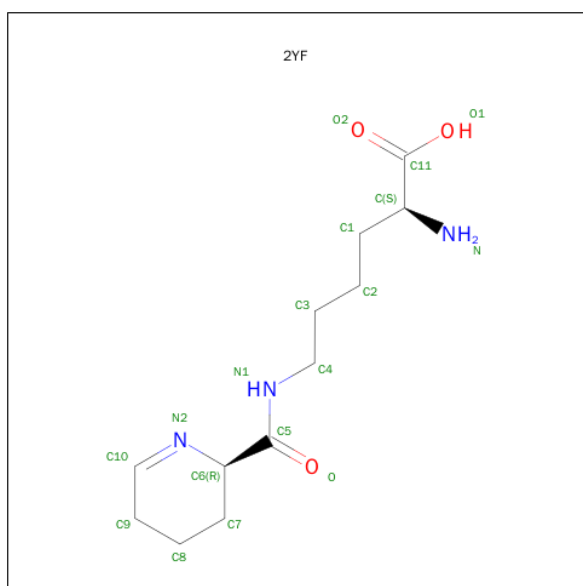
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is N 6 -[(2R)-2,3,4,5-TETRAHYDROPYRIDIN-2-YLCARBONYL]-L-LYSINE (three-letter code: 2YF) (formula: C<sub>12</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	12	3	3		
5	B	1	Total	C	N	O	0	0
			18	12	3	3		
5	C	1	Total	C	N	O	0	0
			18	12	3	3		
5	D	1	Total	C	N	O	0	0
			18	12	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

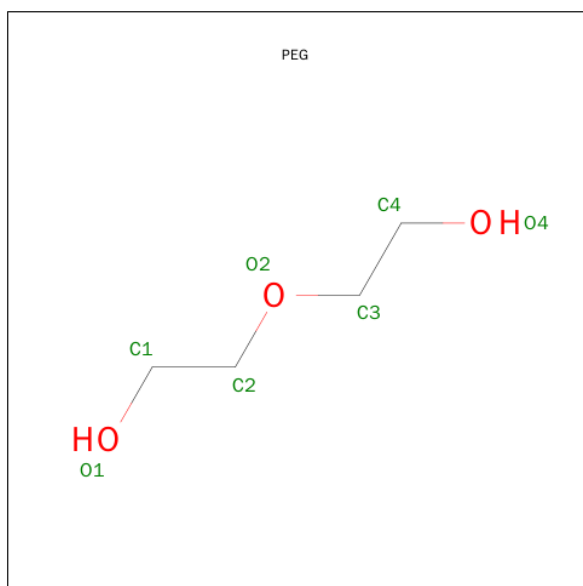
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

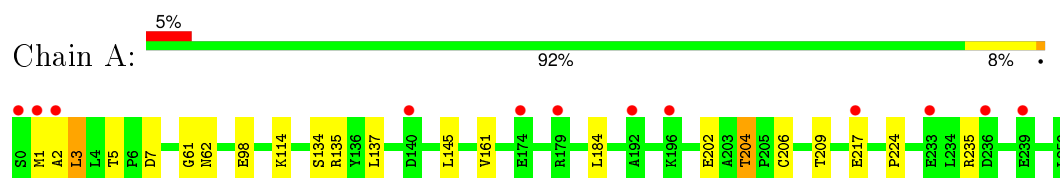
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	149	Total	O	0	0
			149	149		
9	B	134	Total	O	0	0
			134	134		
9	C	34	Total	O	0	0
			34	34		
9	D	31	Total	O	0	0
			31	31		

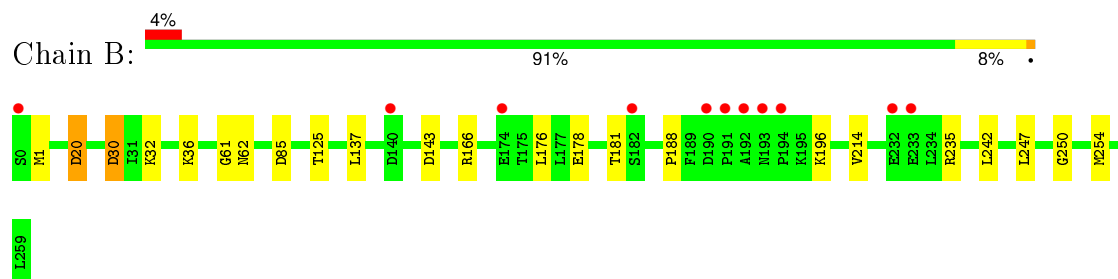
### 3 Residue-property plots [i](#)

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.

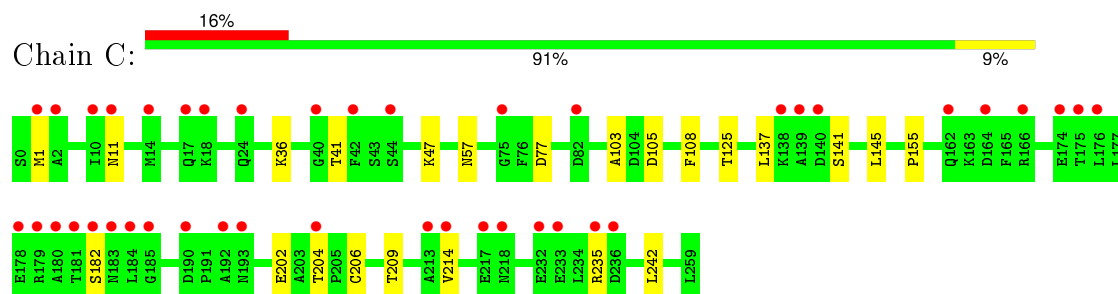
- Molecule 1: PYLD, pyrrollysine synthase



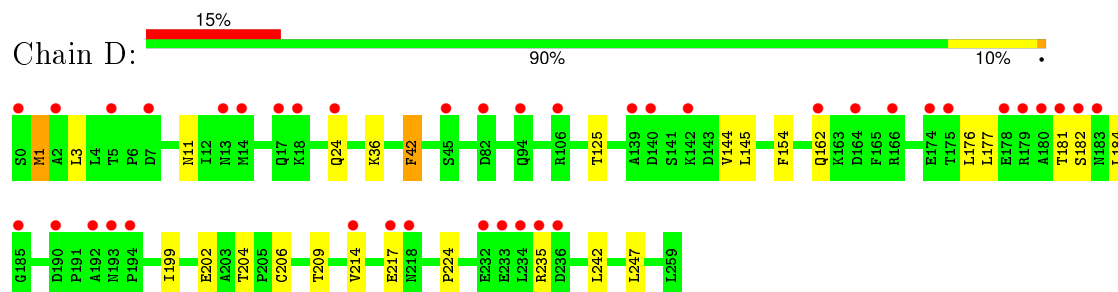
- Molecule 1: PYLD, pyrrollysine synthase



- Molecule 1: PYLD, pyrrollysine synthase



- Molecule 1: PYLD, pyrrollysine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.64Å 261.17Å 48.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (10.00-1.90) 94.5 (10.00-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.183 , 0.222 0.191 , 0.229	Depositor DCC
$R_{free}$ test set	4195 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.48 , 61.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 83914 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: GOL, MG, 2YF, NA, NAI, EDO, PEG

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	0.58	0/1998	0.74	2/2713 (0.1%)
1	B	0.55	0/1998	0.71	1/2713 (0.0%)
1	C	0.35	0/1998	0.55	0/2713
1	D	0.35	0/1998	0.57	0/2713
All	All	0.47	0/7992	0.65	3/10852 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	A	135	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	B	30	ASP	CB-CG-OD1	5.36	123.12	118.30

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	A	1962	0	1956	17	0
1	B	1962	0	1955	11	0
1	C	1962	0	1955	9	0
1	D	1962	0	1956	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	27	4	0
2	B	44	0	27	5	0
2	C	44	0	27	6	0
2	D	44	0	27	5	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
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	18	0	20	4	0
5	B	18	0	20	4	0
5	C	18	0	20	5	0
5	D	18	0	20	4	0
6	A	4	0	6	0	0
6	B	12	0	18	1	0
6	C	8	0	12	0	0
7	A	48	0	64	4	0
7	B	36	0	48	5	0
7	D	6	0	8	0	0
8	B	21	0	30	1	0
9	A	149	0	0	0	0
9	B	134	0	0	0	0
9	C	34	0	0	1	0
9	D	31	0	0	0	0
All	All	8587	0	8196	65	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 4.

All (65) 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)
2:D:901:NAI:H42N	5:D:904:2YF:H17	1.30	1.13
2:D:901:NAI:C4N	5:D:904:2YF:H17	1.92	1.00
1:A:204:THR:HG21	1:A:209:THR:HG21	1.53	0.89
2:A:901:NAI:H42N	5:A:904:2YF:H17	1.56	0.87
2:B:901:NAI:H42N	5:B:904:2YF:H17	1.64	0.79
1:A:161:VAL:HG12	1:B:36:LYS:HE2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:901:NAI:H42N	5:D:904:2YF:C9	2.14	0.75
1:C:57:ASN:OD1	9:C:1019:HOH:O	2.04	0.75
2:C:901:NAI:H42N	5:C:904:2YF:H17	1.67	0.74
2:C:901:NAI:H42N	5:C:904:2YF:C9	2.19	0.72
1:C:204:THR:HG22	1:C:206:CYS:H	1.57	0.70
2:D:901:NAI:C5N	5:D:904:2YF:H17	2.24	0.68
1:A:202:GLU:OE1	1:A:204:THR:HB	1.95	0.66
2:A:901:NAI:C4N	5:A:904:2YF:H17	2.26	0.65
1:A:7:ASP:HB2	7:A:907:GOL:H32	1.78	0.64
1:C:36:LYS:HD2	1:C:41:THR:O	1.98	0.64
2:A:901:NAI:H42N	5:A:904:2YF:C9	2.27	0.64
1:D:204:THR:HG21	1:D:209:THR:HG21	1.81	0.63
1:A:206:CYS:HG	1:D:206:CYS:HG	1.47	0.62
1:A:204:THR:HG22	1:A:206:CYS:H	1.66	0.61
2:B:901:NAI:H42N	5:B:904:2YF:C9	2.32	0.60
1:D:1:MET:HE3	1:D:3:LEU:HD11	1.85	0.59
1:A:184:LEU:HA	7:B:909:GOL:C3	2.33	0.58
1:B:36:LYS:HE3	7:B:909:GOL:O3	2.06	0.56
1:D:204:THR:HG22	1:D:206:CYS:H	1.69	0.56
1:B:196:LYS:HD2	6:B:907:EDO:H12	1.89	0.55
2:B:901:NAI:C4N	5:B:904:2YF:H17	2.36	0.54
1:A:5:THR:HB	7:A:907:GOL:H12	1.91	0.53
1:C:204:THR:HG21	1:C:209:THR:HG21	1.91	0.53
1:A:5:THR:HB	7:A:907:GOL:C1	2.39	0.53
1:A:202:GLU:O	1:A:224:PRO:HD2	2.10	0.52
1:A:98:GLU:HG2	1:A:114:LYS:HE2	1.91	0.52
2:C:901:NAI:C4N	5:C:904:2YF:H17	2.37	0.51
1:A:184:LEU:HA	7:B:909:GOL:H31	1.92	0.50
1:A:184:LEU:HA	7:B:909:GOL:H32	1.93	0.50
2:C:901:NAI:H42N	5:C:904:2YF:H18	1.93	0.50
1:C:125:THR:HG21	2:C:901:NAI:H4N	1.95	0.49
1:A:2:ALA:O	1:A:3:LEU:HD13	2.14	0.48
2:A:901:NAI:C3N	5:A:904:2YF:H17	2.43	0.48
2:C:901:NAI:C4N	5:C:904:2YF:C9	2.91	0.48
1:B:20:ASP:OD1	1:B:30:ASP:HB2	2.14	0.48
1:B:125:THR:HG21	2:B:901:NAI:H4N	1.98	0.46
1:D:125:THR:HG21	2:D:901:NAI:H4N	1.97	0.46
1:D:202:GLU:OE1	1:D:204:THR:HB	2.16	0.46
1:D:36:LYS:HE3	1:D:42:PHE:CZ	2.51	0.45
1:D:202:GLU:O	1:D:224:PRO:HD2	2.16	0.45
1:B:250:GLY:O	1:B:254:MET:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLY:O	1:B:62:ASN:HB2	2.16	0.45
1:A:204:THR:CG2	1:A:206:CYS:HB2	2.47	0.45
1:A:61:GLY:O	1:A:62:ASN:HB2	2.18	0.44
1:D:204:THR:HG22	1:D:206:CYS:N	2.33	0.44
1:B:181:THR:HG21	1:B:188:PRO:HG3	2.00	0.43
1:C:202:GLU:OE1	1:C:204:THR:HB	2.18	0.43
1:B:143:ASP:OD1	1:B:166:ARG:HD2	2.19	0.42
1:C:103:ALA:HB2	1:C:108:PHE:CD1	2.54	0.42
1:D:144:VAL:HG23	1:D:199:ILE:HG22	2.00	0.42
1:B:36:LYS:CE	7:B:909:GOL:O3	2.67	0.42
2:B:901:NAI:C3N	5:B:904:2YF:H17	2.50	0.42
1:A:134:SER:OG	7:A:912:GOL:H11	2.20	0.41
1:D:154:PHE:CZ	1:D:184:LEU:CD1	3.03	0.41
1:C:1:MET:CE	1:C:105:ASP:HB3	2.49	0.41
1:D:36:LYS:CE	1:D:42:PHE:CZ	3.04	0.41
1:D:177:LEU:O	1:D:181:THR:HG23	2.20	0.41
1:B:85:ASP:HA	8:B:915:PEG:H32	2.01	0.41
1:C:47:LYS:HA	1:C:77:ASP:O	2.22	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	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	B	258/260 (99%)	251 (97%)	6 (2%)	1 (0%)	39	27
1	C	258/260 (99%)	248 (96%)	9 (4%)	1 (0%)	39	27
1	D	258/260 (99%)	251 (97%)	6 (2%)	1 (0%)	39	27
All	All	1032/1040 (99%)	997 (97%)	32 (3%)	3 (0%)	46	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	247	LEU
1	C	141	SER
1	D	247	LEU

### 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	215/215 (100%)	208 (97%)	7 (3%)	45	34
1	B	215/215 (100%)	206 (96%)	9 (4%)	36	24
1	C	215/215 (100%)	207 (96%)	8 (4%)	41	29
1	D	215/215 (100%)	203 (94%)	12 (6%)	26	14
All	All	860/860 (100%)	824 (96%)	36 (4%)	36	24

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LEU
1	A	137	LEU
1	A	145	LEU
1	A	204	THR
1	A	217	GLU
1	A	235	ARG
1	B	1	MET
1	B	20	ASP
1	B	32	LYS
1	B	137	LEU
1	B	176	LEU
1	B	178	GLU
1	B	214	VAL
1	B	235	ARG
1	B	242	LEU
1	C	11	ASN
1	C	137	LEU
1	C	145	LEU

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Mol	Chain	Res	Type
1	C	155	PRO
1	C	182	SER
1	C	214	VAL
1	C	235	ARG
1	C	242	LEU
1	D	1	MET
1	D	11	ASN
1	D	24	GLN
1	D	42	PHE
1	D	145	LEU
1	D	162	GLN
1	D	176	LEU
1	D	182	SER
1	D	214	VAL
1	D	217	GLU
1	D	235	ARG
1	D	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	B	162	GLN
1	B	183	ASN
1	B	208	ASN
1	C	11	ASN
1	C	162	GLN
1	D	11	ASN
1	D	57	ASN
1	D	72	GLN
1	D	241	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 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	NAI	A	901	4	38,48,48	1.00	2 (5%)	48,73,73	1.89	9 (18%)
5	2YF	A	904	-	14,18,18	0.60	0	11,22,22	1.39	2 (18%)
6	EDO	A	905	-	3,3,3	0.59	0	2,2,2	0.18	0
7	GOL	A	906	-	5,5,5	0.24	0	5,5,5	0.19	0
7	GOL	A	907	-	5,5,5	0.38	0	5,5,5	0.65	0
7	GOL	A	908	-	5,5,5	0.14	0	5,5,5	0.42	0
7	GOL	A	909	-	5,5,5	0.19	0	5,5,5	0.37	0
7	GOL	A	910	-	5,5,5	0.32	0	5,5,5	0.59	0
7	GOL	A	911	-	5,5,5	0.35	0	5,5,5	0.20	0
7	GOL	A	912	-	5,5,5	0.35	0	5,5,5	0.36	0
7	GOL	A	913	-	5,5,5	0.27	0	5,5,5	0.50	0
2	NAI	B	901	4	38,48,48	1.05	3 (7%)	48,73,73	2.04	10 (20%)
5	2YF	B	904	-	14,18,18	0.82	1 (7%)	11,22,22	1.35	2 (18%)
6	EDO	B	905	-	3,3,3	0.50	0	2,2,2	0.30	0
6	EDO	B	906	-	3,3,3	0.58	0	2,2,2	0.47	0
6	EDO	B	907	-	3,3,3	0.58	0	2,2,2	0.27	0
7	GOL	B	908	-	5,5,5	0.14	0	5,5,5	0.29	0
7	GOL	B	909	-	5,5,5	0.21	0	5,5,5	1.01	0
7	GOL	B	910	-	5,5,5	0.24	0	5,5,5	0.83	0
7	GOL	B	911	-	5,5,5	0.30	0	5,5,5	0.19	0
7	GOL	B	912	-	5,5,5	0.21	0	5,5,5	0.16	0
7	GOL	B	913	-	5,5,5	0.24	0	5,5,5	0.65	0
8	PEG	B	914	-	6,6,6	0.54	0	5,5,5	0.32	0
8	PEG	B	915	-	6,6,6	0.35	0	5,5,5	0.54	0
8	PEG	B	916	-	6,6,6	0.36	0	5,5,5	0.40	0
2	NAI	C	901	4	38,48,48	1.04	2 (5%)	48,73,73	1.68	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	2YF	C	904	-	14,18,18	0.80	0	11,22,22	1.21	1 (9%)
6	EDO	C	905	-	3,3,3	0.60	0	2,2,2	0.16	0
6	EDO	C	906	-	3,3,3	0.46	0	2,2,2	0.50	0
2	NAI	D	901	4	38,48,48	0.97	2 (5%)	48,73,73	1.88	8 (16%)
5	2YF	D	904	-	14,18,18	0.85	1 (7%)	11,22,22	1.61	2 (18%)
7	GOL	D	905	-	5,5,5	0.42	0	5,5,5	0.54	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	NAI	A	901	4	-	0/25/72/72	0/5/5/5
5	2YF	A	904	-	-	0/12/24/24	0/1/1/1
6	EDO	A	905	-	-	0/1/1/1	0/0/0/0
7	GOL	A	906	-	-	0/4/4/4	0/0/0/0
7	GOL	A	907	-	-	0/4/4/4	0/0/0/0
7	GOL	A	908	-	-	0/4/4/4	0/0/0/0
7	GOL	A	909	-	-	0/4/4/4	0/0/0/0
7	GOL	A	910	-	-	0/4/4/4	0/0/0/0
7	GOL	A	911	-	-	0/4/4/4	0/0/0/0
7	GOL	A	912	-	-	0/4/4/4	0/0/0/0
7	GOL	A	913	-	-	0/4/4/4	0/0/0/0
2	NAI	B	901	4	-	0/25/72/72	0/5/5/5
5	2YF	B	904	-	-	0/12/24/24	0/1/1/1
6	EDO	B	905	-	-	0/1/1/1	0/0/0/0
6	EDO	B	906	-	-	0/1/1/1	0/0/0/0
6	EDO	B	907	-	-	0/1/1/1	0/0/0/0
7	GOL	B	908	-	-	0/4/4/4	0/0/0/0
7	GOL	B	909	-	-	0/4/4/4	0/0/0/0
7	GOL	B	910	-	-	0/4/4/4	0/0/0/0
7	GOL	B	911	-	-	0/4/4/4	0/0/0/0
7	GOL	B	912	-	-	0/4/4/4	0/0/0/0
7	GOL	B	913	-	-	0/4/4/4	0/0/0/0
8	PEG	B	914	-	-	0/4/4/4	0/0/0/0
8	PEG	B	915	-	-	0/4/4/4	0/0/0/0
8	PEG	B	916	-	-	0/4/4/4	0/0/0/0
2	NAI	C	901	4	-	0/25/72/72	0/5/5/5
5	2YF	C	904	-	-	0/12/24/24	0/1/1/1
6	EDO	C	905	-	-	0/1/1/1	0/0/0/0
6	EDO	C	906	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	D	901	4	-	0/25/72/72	0/5/5/5
5	2YF	D	904	-	-	0/12/24/24	0/1/1/1
7	GOL	D	905	-	-	0/4/4/4	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	904	2YF	C6-C5	-2.26	1.49	1.53
5	D	904	2YF	C6-C5	-2.12	1.49	1.53
2	B	901	NAI	C2A-N3A	2.11	1.35	1.32
2	A	901	NAI	C6N-C5N	2.57	1.38	1.33
2	D	901	NAI	C5A-C4A	2.77	1.46	1.40
2	C	901	NAI	C5A-C4A	2.86	1.46	1.40
2	B	901	NAI	C6N-C5N	3.07	1.39	1.33
2	B	901	NAI	C5A-C4A	3.15	1.47	1.40
2	C	901	NAI	C6N-C5N	3.20	1.39	1.33
2	D	901	NAI	C6N-C5N	3.23	1.39	1.33
2	A	901	NAI	C5A-C4A	3.30	1.47	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAI	N3A-C2A-N1A	-9.68	121.49	128.89
2	A	901	NAI	N3A-C2A-N1A	-8.43	122.44	128.89
2	C	901	NAI	N3A-C2A-N1A	-8.32	122.53	128.89
2	D	901	NAI	N3A-C2A-N1A	-8.16	122.64	128.89
2	B	901	NAI	C1B-N9A-C4A	-4.09	120.77	126.94
2	A	901	NAI	C4B-O4B-C1B	-4.01	105.31	109.72
5	D	904	2YF	C7-C6-C5	-3.95	103.61	111.89
2	C	901	NAI	PN-O3-PA	-3.78	122.11	132.73
2	D	901	NAI	C1D-N1N-C2N	-3.73	114.41	120.91
2	A	901	NAI	C4A-C5A-N7A	-3.71	106.07	109.48
2	D	901	NAI	PN-O3-PA	-3.70	122.33	132.73
2	B	901	NAI	C4A-C5A-N7A	-3.58	106.19	109.48
2	B	901	NAI	PN-O3-PA	-3.53	122.81	132.73
5	A	904	2YF	C7-C6-C5	-3.35	104.87	111.89
2	D	901	NAI	C4A-C5A-N7A	-3.32	106.42	109.48
2	A	901	NAI	C1B-N9A-C4A	-3.27	122.01	126.94
2	D	901	NAI	C4B-O4B-C1B	-3.09	106.32	109.72
5	B	904	2YF	C7-C6-C5	-3.05	105.49	111.89
2	A	901	NAI	PN-O3-PA	-2.99	124.33	132.73
2	D	901	NAI	C1B-N9A-C4A	-2.95	122.49	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAI	O4D-C1D-N1N	-2.82	102.12	108.07
2	B	901	NAI	C1D-N1N-C2N	-2.79	116.04	120.91
2	A	901	NAI	C1D-N1N-C2N	-2.70	116.21	120.91
2	B	901	NAI	O3-PN-O5D	-2.66	95.88	102.94
5	C	904	2YF	C7-C6-C5	-2.65	106.34	111.89
2	C	901	NAI	C1D-N1N-C2N	-2.62	116.34	120.91
5	A	904	2YF	C7-C8-C9	-2.57	103.97	111.43
2	B	901	NAI	C4B-O4B-C1B	-2.54	106.93	109.72
2	C	901	NAI	C4A-C5A-N7A	-2.27	107.39	109.48
2	C	901	NAI	C1B-N9A-C4A	-2.26	123.53	126.94
5	B	904	2YF	C7-C8-C9	-2.18	105.10	111.43
2	A	901	NAI	C2A-N1A-C6A	2.06	122.44	118.77
2	C	901	NAI	C2A-N1A-C6A	2.14	122.60	118.77
2	B	901	NAI	C2A-N1A-C6A	2.15	122.62	118.77
2	C	901	NAI	C2D-C1D-N1N	2.16	119.18	113.34
2	A	901	NAI	O4B-C1B-N9A	2.18	112.65	108.10
5	D	904	2YF	C8-C9-C10	2.18	117.36	112.27
2	A	901	NAI	C2D-C1D-N1N	2.28	119.49	113.34
2	D	901	NAI	C2D-C1D-N1N	2.28	119.50	113.34
2	B	901	NAI	C2D-C1D-N1N	2.29	119.53	113.34
2	D	901	NAI	O4B-C1B-N9A	2.81	113.98	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAI	4	0
5	A	904	2YF	4	0
7	A	907	GOL	3	0
7	A	912	GOL	1	0
2	B	901	NAI	5	0
5	B	904	2YF	4	0
6	B	907	EDO	1	0
7	B	909	GOL	5	0
8	B	915	PEG	1	0
2	C	901	NAI	6	0
5	C	904	2YF	5	0
2	D	901	NAI	5	0
5	D	904	2YF	4	0

## 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	260/260 (100%)	0.06	12 (4%)	36 39	16, 22, 45, 60	0
1	B	260/260 (100%)	0.15	11 (4%)	40 44	16, 24, 51, 81	0
1	C	260/260 (100%)	0.73	42 (16%)	3 3	33, 46, 71, 87	0
1	D	260/260 (100%)	0.78	40 (15%)	3 3	35, 47, 69, 83	0
All	All	1040/1040 (100%)	0.43	105 (10%)	9 10	16, 39, 66, 87	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	ALA	9.0
1	D	192	ALA	7.6
1	D	193	ASN	7.3
1	B	193	ASN	6.5
1	D	140	ASP	5.2
1	D	164	ASP	4.8
1	C	178	GLU	4.4
1	C	180	ALA	4.3
1	C	140	ASP	4.2
1	C	42	PHE	4.1
1	D	236	ASP	4.0
1	D	0	SER	3.9
1	C	235	ARG	3.9
1	C	192	ALA	3.9
1	C	179	ARG	3.8
1	C	181	THR	3.8
1	C	232	GLU	3.8
1	D	218	ASN	3.8
1	B	194	PRO	3.7
1	D	182	SER	3.7
1	A	140	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	180	ALA	3.6
1	A	0	SER	3.5
1	D	179	ARG	3.5
1	C	176	LEU	3.5
1	D	2	ALA	3.5
1	C	14	MET	3.5
1	C	164	ASP	3.4
1	C	236	ASP	3.3
1	C	82	ASP	3.3
1	D	17	GLN	3.2
1	C	166	ARG	3.1
1	D	178	GLU	3.1
1	C	213	ALA	3.1
1	B	140	ASP	3.1
1	D	14	MET	3.0
1	C	183	ASN	3.0
1	C	18	LYS	3.0
1	A	174	GLU	2.9
1	C	174	GLU	2.9
1	D	142	LYS	2.9
1	D	233	GLU	2.9
1	D	183	ASN	2.9
1	D	185	GLY	2.9
1	C	138	LYS	2.8
1	C	233	GLU	2.8
1	D	106	ARG	2.8
1	D	234	LEU	2.8
1	D	194	PRO	2.8
1	D	232	GLU	2.8
1	C	11	ASN	2.8
1	C	182	SER	2.8
1	D	174	GLU	2.7
1	D	18	LYS	2.7
1	B	233	GLU	2.7
1	A	192	ALA	2.7
1	D	235	ARG	2.7
1	D	190	ASP	2.7
1	C	184	LEU	2.6
1	C	2	ALA	2.6
1	C	17	GLN	2.6
1	B	0	SER	2.6
1	C	162	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	193	ASN	2.5
1	B	232	GLU	2.5
1	C	217	GLU	2.5
1	D	166	ARG	2.5
1	C	44	SER	2.5
1	B	191	PRO	2.5
1	A	179	ARG	2.5
1	B	182	SER	2.4
1	C	24	GLN	2.4
1	C	75	GLY	2.4
1	D	175	THR	2.4
1	C	185	GLY	2.4
1	D	45	SER	2.4
1	B	174	GLU	2.3
1	D	94	GLN	2.3
1	D	162	GLN	2.3
1	D	82	ASP	2.3
1	C	218	ASN	2.3
1	D	214	VAL	2.2
1	A	236	ASP	2.2
1	D	24	GLN	2.2
1	C	175	THR	2.2
1	C	10	ILE	2.2
1	A	196	LYS	2.1
1	D	181	THR	2.1
1	A	1	MET	2.1
1	C	214	VAL	2.1
1	A	239	GLU	2.1
1	D	13	ASN	2.1
1	C	40	GLY	2.1
1	A	233	GLU	2.1
1	C	190	ASP	2.1
1	B	190	ASP	2.1
1	C	204	THR	2.1
1	D	5	THR	2.1
1	C	139	ALA	2.1
1	D	139	ALA	2.1
1	A	217	GLU	2.1
1	D	217	GLU	2.1
1	C	1	MET	2.0
1	D	7	ASP	2.0
1	A	2	ALA	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
7	GOL	B	909	6/6	0.88	0.23	11.34	32,34,35,36	0
6	EDO	B	905	4/4	0.73	0.27	9.96	57,57,59,61	0
7	GOL	A	912	6/6	0.82	0.25	7.01	58,59,62,64	0
7	GOL	A	906	6/6	0.78	0.29	5.94	50,57,60,62	0
7	GOL	B	908	6/6	0.82	0.20	4.54	33,43,49,51	0
6	EDO	A	905	4/4	0.66	0.30	4.37	37,43,44,47	0
4	MG	D	903	1/1	0.93	0.17	3.91	54,54,54,54	0
3	NA	A	902	1/1	0.95	0.20	3.80	35,35,35,35	0
7	GOL	A	910	6/6	0.89	0.21	3.11	41,48,50,50	0
7	GOL	B	910	6/6	0.89	0.15	3.08	39,42,45,51	0
3	NA	C	902	1/1	0.93	0.20	2.53	47,47,47,47	0
3	NA	B	902	1/1	0.95	0.14	2.44	38,38,38,38	0
7	GOL	A	911	6/6	0.72	0.30	2.29	58,61,62,65	0
8	PEG	B	916	7/7	0.94	0.13	2.16	42,43,45,46	0
8	PEG	B	915	7/7	0.89	0.14	2.15	37,39,43,43	0
6	EDO	B	907	4/4	0.76	0.28	2.01	45,46,48,48	0
4	MG	C	903	1/1	0.95	0.14	1.96	50,50,50,50	0
7	GOL	B	913	6/6	0.74	0.20	1.93	35,42,48,54	0
7	GOL	A	908	6/6	0.74	0.21	1.91	40,42,45,46	0
6	EDO	C	906	4/4	0.93	0.21	1.66	40,41,43,44	0
6	EDO	B	906	4/4	0.86	0.18	1.63	31,34,35,39	0
8	PEG	B	914	7/7	0.79	0.21	1.60	39,41,49,54	0
7	GOL	A	913	6/6	0.83	0.16	1.35	38,45,47,54	0
7	GOL	D	905	6/6	0.82	0.16	1.16	43,45,48,48	0
4	MG	A	903	1/1	0.99	0.11	0.82	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	C	905	4/4	0.77	0.20	0.79	47,50,51,51	0
3	NA	D	902	1/1	0.98	0.13	0.51	43,43,43,43	0
5	2YF	D	904	18/18	0.84	0.15	0.28	36,41,45,46	0
5	2YF	C	904	18/18	0.89	0.12	0.18	33,39,47,47	0
7	GOL	B	911	6/6	0.94	0.10	0.12	23,25,26,29	0
4	MG	B	903	1/1	1.00	0.08	-0.03	25,25,25,25	0
5	2YF	A	904	18/18	0.94	0.09	-0.26	18,22,25,26	0
5	2YF	B	904	18/18	0.96	0.09	-0.40	19,22,27,28	0
2	NAI	C	901	44/44	0.94	0.10	-0.52	36,40,46,48	0
7	GOL	A	909	6/6	0.90	0.08	-0.63	56,57,57,58	0
2	NAI	B	901	44/44	0.97	0.08	-0.75	20,25,32,34	0
2	NAI	A	901	44/44	0.97	0.08	-0.83	19,23,30,32	0
2	NAI	D	901	44/44	0.97	0.08	-1.05	34,38,41,44	0
7	GOL	A	907	6/6	0.56	0.58	-	49,55,58,58	0
7	GOL	B	912	6/6	0.81	0.20	-	57,59,61,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.