



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 10:01 PM EDT

PDB ID : 1RLO  
Title : Phospho-aspartyl Intermediate Analogue of ybiV from E. coli K12  
Authors : Roberts, A.; Lee, S.Y.; McCullagh, E.; Silversmith, R.E.; Wemmer, D.E.  
Deposited on : 2003-11-26  
Resolution : 2.00 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

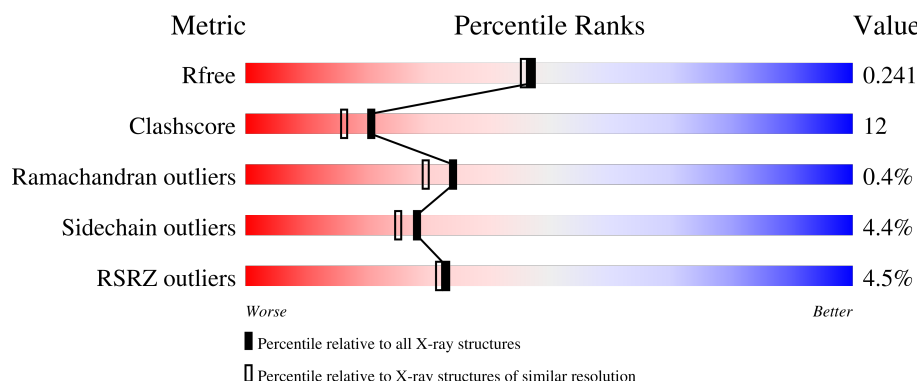
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	271	<div> <div>3%</div> <div>76%</div> <div>21%</div> <div>...</div> </div>
1	B	271	<div> <div>7%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	C	271	<div> <div>2%</div> <div>70%</div> <div>28%</div> <div>..</div> </div>
1	D	271	<div> <div>6%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	BFD	A	9	-	-	X	-
3	GOL	C	805	-	X	-	-
3	GOL	D	806	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9003 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 Phosphatase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	268	Total	Be	C	F	N	O	S		0	0	0
			2133	1	1366	3	361	394	8				
1	B	268	Total	Be	C	F	N	O	S		0	0	0
			2133	1	1366	3	361	394	8				
1	C	268	Total	Be	C	F	N	O	S		0	0	0
			2133	1	1366	3	361	394	8				
1	D	268	Total	Be	C	F	N	O	S		0	0	0
			2133	1	1366	3	361	394	8				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P75792
A	9	BFD	ASP	modified residue	UNP P75792
A	267	TYR	SER	engineered mutation	UNP P75792
B	2	ALA	SER	engineered mutation	UNP P75792
B	9	BFD	ASP	modified residue	UNP P75792
B	267	TYR	SER	engineered mutation	UNP P75792
C	2	ALA	SER	engineered mutation	UNP P75792
C	9	BFD	ASP	modified residue	UNP P75792
C	267	TYR	SER	engineered mutation	UNP P75792
D	2	ALA	SER	engineered mutation	UNP P75792
D	9	BFD	ASP	modified residue	UNP P75792
D	267	TYR	SER	engineered mutation	UNP P75792

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

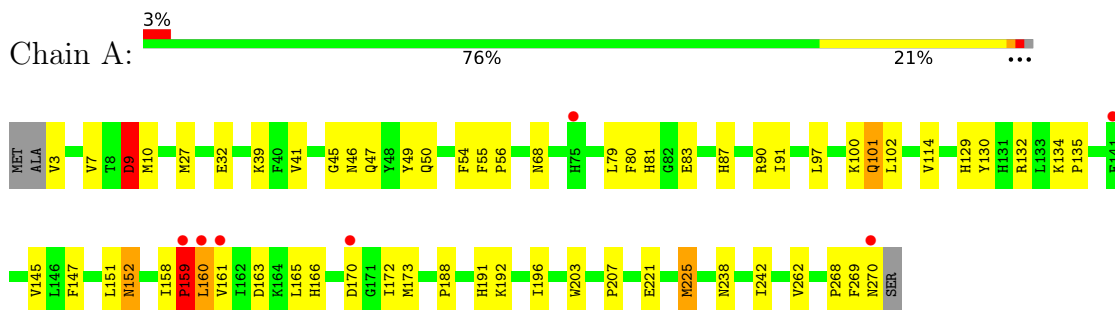
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		
4	B	101	Total	O	0	0
			101	101		
4	C	113	Total	O	0	0
			113	113		
4	D	103	Total	O	0	0
			103	103		

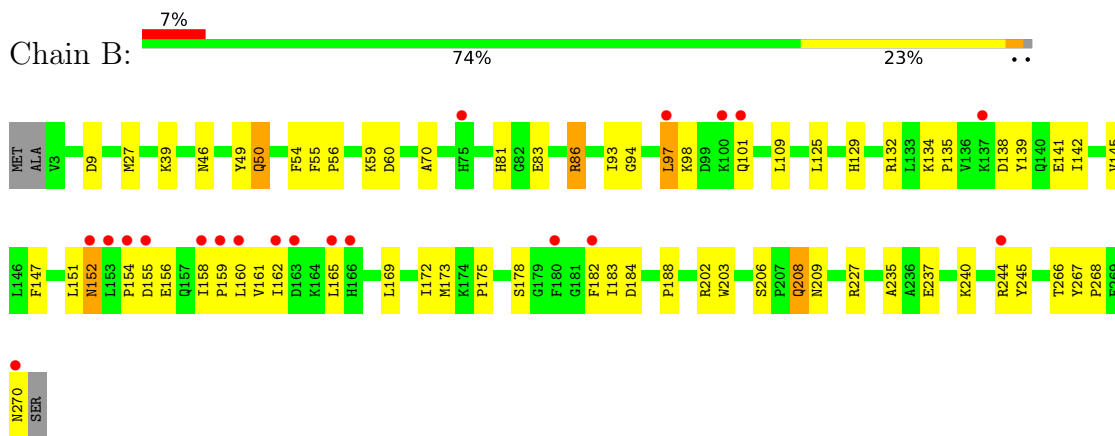
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

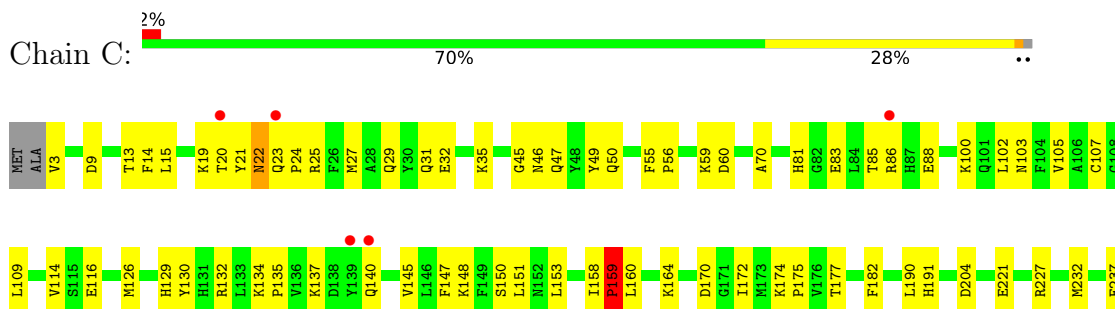
- Molecule 1: Phosphatase

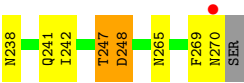


- Molecule 1: Phosphatase

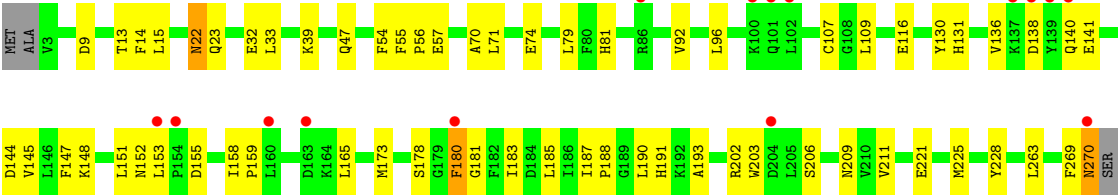
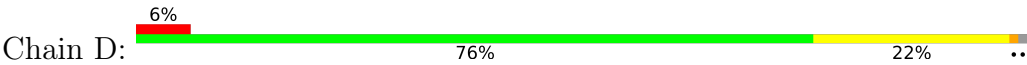


- Molecule 1: Phosphatase





● Molecule 1: Phosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.28Å 91.19Å 176.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 2.00 47.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.85-2.00) 98.7 (47.37-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.29 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.251 0.211 , 0.241	Depositor DCC
$R_{free}$ test set	7906 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BFD, GOL

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	0.38	0/2165	0.66	1/2925 (0.0%)
1	B	0.34	0/2165	0.62	1/2925 (0.0%)
1	C	0.34	0/2165	0.61	1/2925 (0.0%)
1	D	0.34	0/2165	0.57	0/2925
All	All	0.35	0/8660	0.62	3/11700 (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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	PRO	CA-N-CD	-12.75	93.65	111.50
1	A	159	PRO	CA-N-CD	-12.46	94.05	111.50
1	C	159	PRO	CA-N-CD	-11.42	95.51	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	9	BFD	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	2133	0	2118	65	0
1	B	2133	0	2118	50	0
1	C	2133	0	2118	65	0
1	D	2133	0	2118	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	6	0	4	2	0
3	D	6	0	4	1	0
4	A	138	0	0	3	0
4	B	101	0	0	3	0
4	C	113	0	0	3	0
4	D	103	0	0	2	0
All	All	9003	0	8480	210	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 12.

All (210) 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:9:BFD:CB	1:A:9:BFD:CA	1.79	1.56
1:A:9:BFD:CB	1:A:9:BFD:C	2.34	1.04
1:A:9:BFD:CB	1:A:9:BFD:N	2.35	0.88
1:D:269:PHE:O	1:D:270:ASN:HB2	1.72	0.86
1:A:81:HIS:H	1:C:86:ARG:HH21	1.22	0.84
1:C:191:HIS:CG	1:C:221:GLU:HG3	2.16	0.81
1:A:191:HIS:CG	1:A:221:GLU:HG3	2.17	0.80
1:B:83:GLU:HG3	1:B:145:VAL:HG13	1.66	0.78
1:A:160:LEU:C	1:A:160:LEU:HD23	2.05	0.77
1:C:13:THR:HG22	1:C:14:PHE:N	1.99	0.77
1:A:9:BFD:C	1:A:9:BFD:CG	2.64	0.75
1:C:140:GLN:HA	1:C:140:GLN:NE2	2.04	0.73
1:B:50:GLN:HG2	1:B:129:HIS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:SER:H	1:B:209:ASN:HD22	1.36	0.71
1:A:207:PRO:HB3	1:A:225:MET:HE2	1.74	0.70
1:A:262:VAL:HG22	1:A:269:PHE:CZ	2.26	0.70
1:B:169:LEU:O	1:B:172:ILE:HG12	1.92	0.70
1:C:160:LEU:O	1:C:164:LYS:HG3	1.91	0.69
1:B:160:LEU:HD13	1:B:160:LEU:O	1.92	0.69
1:C:132:ARG:HD2	1:D:23:GLN:OE1	1.91	0.69
1:C:237:GLU:O	1:C:241:GLN:HG3	1.91	0.69
1:C:83:GLU:HG3	1:C:145:VAL:HG13	1.75	0.67
1:A:166:HIS:O	1:A:170:ASP:HA	1.94	0.67
1:B:154:PRO:HB2	1:B:156:GLU:HG2	1.78	0.66
1:D:180:PHE:HB3	4:D:907:HOH:O	1.95	0.66
1:B:152:ASN:HD22	1:B:182:PHE:HE1	1.44	0.66
1:A:160:LEU:HG	1:A:160:LEU:O	1.96	0.65
1:B:158:ILE:HA	1:B:161:VAL:HG12	1.79	0.64
1:B:266:THR:OG1	4:B:903:HOH:O	2.15	0.64
1:B:93:ILE:HD13	1:B:139:TYR:HB3	1.79	0.64
1:C:269:PHE:O	1:C:270:ASN:HB2	1.97	0.64
1:A:80:PHE:CD1	1:C:86:ARG:NH2	2.67	0.63
1:A:102:LEU:HD12	1:A:152:ASN:ND2	2.13	0.62
1:C:25:ARG:O	1:C:29:GLN:HG3	1.99	0.62
1:A:81:HIS:H	1:C:86:ARG:NH2	1.95	0.62
1:A:100:LYS:HE2	1:A:100:LYS:HA	1.82	0.60
1:C:49:TYR:CG	1:C:132:ARG:HD3	2.36	0.60
1:A:269:PHE:O	1:A:270:ASN:HB2	2.02	0.60
1:A:158:ILE:HB	1:A:159:PRO:HD2	1.83	0.60
1:C:172:ILE:N	1:C:172:ILE:HD12	2.17	0.60
1:A:81:HIS:CE1	1:C:86:ARG:HG3	2.37	0.60
1:B:55:PHE:N	1:B:56:PRO:HD3	2.18	0.59
1:D:13:THR:HG22	1:D:14:PHE:N	2.17	0.59
1:A:101:GLN:NE2	1:A:101:GLN:N	2.50	0.58
1:C:238:ASN:O	1:C:242:ILE:HG12	2.03	0.58
1:C:150:SER:C	1:C:151:LEU:HD12	2.24	0.57
1:B:178:SER:HA	1:B:184:ASP:OD2	2.05	0.57
1:B:206:SER:H	1:B:209:ASN:ND2	2.03	0.57
1:C:227:ARG:HG3	1:C:227:ARG:HH11	1.70	0.57
1:D:158:ILE:HG23	1:D:183:ILE:HD11	1.87	0.57
1:C:45:GLY:HA3	3:C:805:GOL:O3	2.04	0.56
1:D:74:GLU:OE2	1:D:202:ARG:HD3	2.05	0.56
1:C:158:ILE:HB	1:C:159:PRO:HD2	1.88	0.56
1:A:9:BFD:CA	1:A:9:BFD:CG	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HG12	1:A:165:LEU:CD1	2.36	0.56
1:C:140:GLN:HA	1:C:140:GLN:HE21	1.70	0.56
1:D:79:LEU:HD21	1:D:202:ARG:HD2	1.87	0.56
1:A:158:ILE:O	1:A:161:VAL:N	2.36	0.55
1:A:101:GLN:H	1:A:101:GLN:HE21	1.54	0.54
1:D:79:LEU:HD11	1:D:202:ARG:HD2	1.88	0.54
1:A:160:LEU:O	1:A:160:LEU:CG	2.55	0.54
1:A:80:PHE:HA	1:C:86:ARG:NH2	2.22	0.54
1:B:138:ASP:OD2	1:B:141:GLU:HG3	2.07	0.54
1:C:46:ASN:OD1	1:C:129:HIS:HD2	1.90	0.54
1:B:208:GLN:NE2	1:B:227:ARG:HG2	2.22	0.53
1:A:160:LEU:HD23	1:A:161:VAL:N	2.24	0.53
1:B:161:VAL:HG22	1:B:165:LEU:HG	1.91	0.53
1:C:221:GLU:CD	1:C:221:GLU:H	2.11	0.53
1:C:31:GLN:HA	1:C:31:GLN:NE2	2.22	0.53
1:D:70:ALA:O	1:D:81:HIS:HA	2.09	0.53
1:A:269:PHE:O	1:A:270:ASN:CB	2.56	0.53
1:B:151:LEU:O	1:B:182:PHE:HD1	1.92	0.53
1:B:59:LYS:HE3	4:B:880:HOH:O	2.09	0.52
1:A:161:VAL:HG12	1:A:165:LEU:HD12	1.90	0.52
1:D:158:ILE:HB	1:D:159:PRO:HD3	1.92	0.52
1:A:46:ASN:OD1	1:A:129:HIS:HD2	1.93	0.52
1:B:227:ARG:HD2	1:B:244:ARG:NH1	2.25	0.52
1:A:83:GLU:HG2	1:A:145:VAL:HB	1.92	0.52
1:C:19:LYS:N	1:C:19:LYS:HD2	2.24	0.51
1:C:102:LEU:HD11	1:C:151:LEU:HD23	1.92	0.51
1:D:138:ASP:OD2	1:D:140:GLN:HB2	2.11	0.51
1:D:158:ILE:HD11	1:D:181:GLY:HA2	1.91	0.51
1:A:45:GLY:HA2	1:A:68:ASN:N	2.25	0.51
1:A:101:GLN:N	1:A:101:GLN:HE21	2.07	0.51
1:A:87:HIS:O	1:A:91:ILE:HG13	2.11	0.51
1:C:177:THR:HG22	4:C:878:HOH:O	2.09	0.51
1:B:59:LYS:HE2	1:B:60:ASP:OD1	2.10	0.50
1:C:153:LEU:HD23	1:C:153:LEU:N	2.26	0.50
1:D:187:ILE:HB	1:D:190:LEU:HD12	1.93	0.50
1:B:94:GLY:O	1:B:98:LYS:HG3	2.12	0.50
1:A:81:HIS:HE1	1:C:86:ARG:HG3	1.77	0.50
1:B:39:LYS:HD3	1:B:203:TRP:CE2	2.47	0.50
1:A:49:TYR:CG	1:A:132:ARG:HD3	2.47	0.49
1:C:151:LEU:HD12	1:C:151:LEU:N	2.26	0.49
1:A:46:ASN:OD1	1:A:129:HIS:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:HB2	4:A:893:HOH:O	2.11	0.49
1:D:22:ASN:C	1:D:22:ASN:HD22	2.15	0.49
1:A:221:GLU:CD	1:A:221:GLU:H	2.16	0.49
1:D:55:PHE:N	1:D:56:PRO:HD3	2.28	0.49
1:A:192:LYS:O	1:A:196:ILE:HG13	2.11	0.49
1:C:102:LEU:HD21	1:C:151:LEU:HG	1.94	0.49
1:A:45:GLY:HA2	1:A:68:ASN:H	1.78	0.49
1:C:107:CYS:SG	1:C:148:LYS:HE2	2.53	0.49
1:B:125:LEU:HD21	1:B:182:PHE:CE2	2.48	0.49
1:C:85:THR:OG1	1:C:88:GLU:HG3	2.12	0.48
1:D:191:HIS:CE1	1:D:193:ALA:HB3	2.47	0.48
1:A:191:HIS:ND1	1:A:221:GLU:HG3	2.27	0.48
1:D:152:ASN:HA	1:D:181:GLY:O	2.13	0.48
1:C:22:ASN:OD1	1:C:24:PRO:HD2	2.12	0.48
1:A:79:LEU:O	1:A:79:LEU:HD23	2.13	0.48
1:A:268:PRO:HD2	1:A:269:PHE:CD1	2.49	0.48
1:B:227:ARG:HD2	1:B:244:ARG:HH12	1.78	0.48
1:A:207:PRO:HA	1:A:225:MET:HE3	1.95	0.48
1:A:7:VAL:HG22	1:A:41:VAL:HB	1.95	0.48
1:C:49:TYR:CD1	1:C:132:ARG:HD3	2.48	0.48
1:C:221:GLU:HG2	4:C:823:HOH:O	2.13	0.48
1:D:107:CYS:SG	1:D:148:LYS:HE2	2.54	0.48
1:D:54:PHE:C	1:D:56:PRO:HD3	2.33	0.48
1:B:139:TYR:O	1:B:142:ILE:HG13	2.13	0.48
1:A:87:HIS:CD2	1:A:90:ARG:HH21	2.32	0.48
1:C:55:PHE:N	1:C:56:PRO:HD3	2.29	0.47
1:B:93:ILE:HG22	1:B:97:LEU:HD22	1.95	0.47
1:B:208:GLN:HE21	1:B:208:GLN:CA	2.27	0.47
1:A:49:TYR:CD1	1:A:132:ARG:HD3	2.49	0.47
1:C:32:GLU:OE1	1:C:35:LYS:HD2	2.14	0.47
1:D:144:ASP:OD2	1:D:145:VAL:N	2.48	0.47
1:A:158:ILE:HG22	1:A:159:PRO:CD	2.45	0.47
1:B:46:ASN:HB3	1:B:50:GLN:CG	2.44	0.47
1:B:158:ILE:N	1:B:159:PRO:CD	2.77	0.47
1:C:20:THR:HG22	1:C:21:TYR:N	2.29	0.47
1:C:116:GLU:OE1	1:C:137:LYS:HG2	2.14	0.47
1:B:267:TYR:CD1	1:B:268:PRO:HA	2.50	0.47
1:A:3:VAL:N	4:A:815:HOH:O	2.48	0.47
1:A:238:ASN:O	1:A:242:ILE:HG13	2.16	0.46
1:B:54:PHE:C	1:B:56:PRO:HD3	2.35	0.46
1:B:158:ILE:O	1:B:162:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:N	1:C:24:PRO:CD	2.79	0.46
1:D:211:VAL:HG22	1:D:228:TYR:HB2	1.97	0.46
1:B:158:ILE:HA	1:B:161:VAL:CG1	2.46	0.46
1:C:182:PHE:HB3	3:C:805:GOL:O2	2.16	0.46
1:D:39:LYS:HD3	1:D:203:TRP:CE3	2.50	0.46
1:A:221:GLU:HG2	4:A:807:HOH:O	2.15	0.46
1:C:170:ASP:O	1:C:172:ILE:HD12	2.16	0.46
1:D:116:GLU:HA	4:D:906:HOH:O	2.16	0.45
1:C:102:LEU:HD21	1:C:151:LEU:CG	2.46	0.45
1:A:55:PHE:N	1:A:56:PRO:HD3	2.32	0.45
1:C:102:LEU:HD21	1:C:151:LEU:HD23	1.98	0.45
1:B:208:GLN:HE22	1:B:227:ARG:HG2	1.80	0.45
1:C:13:THR:CG2	1:C:14:PHE:N	2.66	0.45
1:C:134:LYS:HA	1:C:135:PRO:HD3	1.87	0.45
1:A:172:ILE:HG22	1:A:173:MET:HG3	1.99	0.45
1:C:102:LEU:HD23	1:C:103:ASN:N	2.32	0.45
1:D:165:LEU:HD13	1:D:185:LEU:HD21	1.97	0.45
1:A:79:LEU:HD23	1:A:79:LEU:C	2.38	0.44
1:C:191:HIS:ND1	1:C:221:GLU:HG3	2.33	0.44
1:B:172:ILE:HG22	1:B:173:MET:HG3	2.00	0.44
1:D:138:ASP:OD2	1:D:141:GLU:HG2	2.17	0.44
1:C:47:GLN:HB2	1:C:130:TYR:CD2	2.53	0.44
1:D:206:SER:H	1:D:209:ASN:HD22	1.63	0.44
1:B:152:ASN:ND2	1:B:182:PHE:HE1	2.11	0.44
1:D:92:VAL:O	1:D:96:LEU:HG	2.17	0.44
1:C:247:THR:OG1	1:C:248:ASP:N	2.50	0.44
1:D:116:GLU:HG2	1:D:136:VAL:O	2.18	0.44
1:B:125:LEU:HD21	1:B:182:PHE:HE2	1.83	0.44
1:C:70:ALA:O	1:C:81:HIS:HA	2.17	0.44
1:A:102:LEU:HD11	1:A:151:LEU:HB3	2.00	0.43
1:B:27:MET:HB2	4:B:865:HOH:O	2.18	0.43
1:C:174:LYS:HA	1:C:175:PRO:HD3	1.86	0.43
1:B:158:ILE:HB	1:B:159:PRO:HD3	2.00	0.43
1:A:158:ILE:CB	1:A:159:PRO:HD2	2.47	0.43
1:C:59:LYS:NZ	1:C:60:ASP:OD1	2.51	0.43
1:A:161:VAL:CG1	1:A:165:LEU:CD1	2.96	0.43
1:D:13:THR:CG2	1:D:14:PHE:N	2.77	0.43
1:A:47:GLN:HB2	1:A:130:TYR:CD2	2.54	0.42
1:B:49:TYR:CD1	1:B:132:ARG:HD3	2.54	0.42
1:D:173:MET:HA	1:D:188:PRO:HD3	2.00	0.42
1:D:47:GLN:HB2	1:D:130:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:CB	1:B:156:GLU:HG2	2.49	0.42
1:B:165:LEU:HD13	1:B:175:PRO:HG3	2.01	0.42
1:C:269:PHE:C	1:C:270:ASN:HD22	2.22	0.42
1:B:235:ALA:O	1:B:240:LYS:HE3	2.19	0.42
1:C:3:VAL:N	4:C:821:HOH:O	2.52	0.42
1:D:191:HIS:CD2	1:D:221:GLU:HG2	2.54	0.42
1:B:93:ILE:O	1:B:97:LEU:HB2	2.19	0.42
1:D:178:SER:OG	3:D:806:GOL:O2	2.35	0.42
1:A:173:MET:HA	1:A:188:PRO:HD3	2.01	0.42
1:C:102:LEU:HD21	1:C:151:LEU:CD2	2.49	0.41
1:B:155:ASP:HA	1:B:183:ILE:HG12	2.02	0.41
1:C:13:THR:HA	1:C:232:MET:HG3	2.01	0.41
1:C:59:LYS:HE3	1:D:57:GLU:HG2	2.01	0.41
1:D:151:LEU:N	1:D:151:LEU:HD12	2.35	0.41
1:B:70:ALA:O	1:B:81:HIS:HA	2.19	0.41
1:C:31:GLN:HA	1:C:31:GLN:HE21	1.84	0.41
1:A:54:PHE:C	1:A:56:PRO:HD3	2.41	0.41
1:A:262:VAL:CG2	1:A:269:PHE:CZ	2.99	0.41
1:B:49:TYR:CG	1:B:132:ARG:HD3	2.56	0.41
1:B:245:TYR:CE2	1:B:268:PRO:HB3	2.56	0.41
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.86	0.41
1:D:33:LEU:HD23	1:D:263:LEU:HD21	2.01	0.41
1:A:39:LYS:HD3	1:A:203:TRP:CE2	2.56	0.41
1:B:134:LYS:HA	1:B:135:PRO:HD3	1.89	0.41
1:A:134:LYS:HA	1:A:135:PRO:HD3	1.82	0.41
1:C:105:VAL:HG13	1:C:126:MET:HE2	2.02	0.41
1:D:79:LEU:HD13	1:D:202:ARG:NH1	2.36	0.41
1:C:59:LYS:HE3	1:D:57:GLU:CG	2.51	0.41
1:A:114:VAL:O	1:A:135:PRO:HA	2.21	0.40
1:B:86:ARG:NH1	1:B:86:ARG:HG3	2.36	0.40
1:A:9:BFD:CG	1:A:10:MET:N	2.85	0.40
1:D:155:ASP:OD2	1:D:180:PHE:CD2	2.74	0.40
1:C:114:VAL:O	1:C:135:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	265/271 (98%)	255 (96%)	10 (4%)	0	100	100
1	B	265/271 (98%)	253 (96%)	11 (4%)	1 (0%)	34	30
1	C	265/271 (98%)	249 (94%)	14 (5%)	2 (1%)	19	13
1	D	265/271 (98%)	252 (95%)	12 (4%)	1 (0%)	34	30
All	All	1060/1084 (98%)	1009 (95%)	47 (4%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	GLN
1	C	22	ASN
1	C	100	LYS
1	D	180	PHE

### 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	227/229 (99%)	217 (96%)	10 (4%)	28	25
1	B	227/229 (99%)	217 (96%)	10 (4%)	28	25
1	C	227/229 (99%)	217 (96%)	10 (4%)	28	25
1	D	227/229 (99%)	217 (96%)	10 (4%)	28	25
All	All	908/916 (99%)	868 (96%)	40 (4%)	28	25



All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	MET
1	A	32	GLU
1	A	50	GLN
1	A	97	LEU
1	A	101	GLN
1	A	147	PHE
1	A	152	ASN
1	A	159	PRO
1	A	160	LEU
1	A	225	MET
1	B	50	GLN
1	B	86	ARG
1	B	97	LEU
1	B	109	LEU
1	B	147	PHE
1	B	152	ASN
1	B	202	ARG
1	B	208	GLN
1	B	237	GLU
1	B	270	ASN
1	C	15	LEU
1	C	27	MET
1	C	50	GLN
1	C	109	LEU
1	C	147	PHE
1	C	159	PRO
1	C	204	ASP
1	C	247	THR
1	C	248	ASP
1	C	265	ASN
1	D	15	LEU
1	D	22	ASN
1	D	32	GLU
1	D	71	LEU
1	D	109	LEU
1	D	131	HIS
1	D	147	PHE
1	D	153	LEU
1	D	225	MET
1	D	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	50	GLN
1	A	78	GLN
1	A	101	GLN
1	A	110	GLN
1	A	129	HIS
1	A	152	ASN
1	A	208	GLN
1	A	265	ASN
1	B	50	GLN
1	B	78	GLN
1	B	103	ASN
1	B	152	ASN
1	B	157	GLN
1	B	208	GLN
1	B	209	ASN
1	B	241	GLN
1	C	31	GLN
1	C	50	GLN
1	C	78	GLN
1	C	129	HIS
1	C	140	GLN
1	C	270	ASN
1	D	22	ASN
1	D	131	HIS
1	D	152	ASN
1	D	209	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	BFD	C	9	1,2	8,11,12	0.85	0	3,15,17	2.32	1 (33%)
1	BFD	D	9	1,2	8,11,12	0.78	0	3,15,17	2.42	1 (33%)
1	BFD	B	9	1,2	8,11,12	0.75	0	3,15,17	2.37	1 (33%)
1	BFD	A	9	1,2	8,11,12	4.87	3 (37%)	3,15,17	8.46	2 (66%)

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
1	BFD	C	9	1,2	-	0/5/11/13	-
1	BFD	D	9	1,2	-	0/5/11/13	-
1	BFD	B	9	1,2	-	0/5/11/13	-
1	BFD	A	9	1,2	-	1/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	BFD	CB-CA	12.01	1.79	1.53
1	A	9	BFD	CA-N	-5.08	1.32	1.48
1	A	9	BFD	O-C	4.14	1.36	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	BFD	CB-CA-C	-14.07	85.10	111.47
1	D	9	BFD	OD2-CG-CB	-4.18	115.49	124.73
1	A	9	BFD	OD2-CG-CB	-4.11	115.66	124.73
1	B	9	BFD	OD2-CG-CB	-4.10	115.67	124.73
1	C	9	BFD	OD2-CG-CB	-4.01	115.87	124.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	9	BFD	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	9	BFD	6	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
3	GOL	D	806	-	5,5,5	4.66	5 (100%)	5,5,5	5.68	3 (60%)
3	GOL	C	805	-	5,5,5	4.67	5 (100%)	5,5,5	5.75	3 (60%)

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
3	GOL	D	806	-	-	2/4/4/4	-
3	GOL	C	805	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	805	GOL	C3-C2	-7.86	1.19	1.51
3	D	806	GOL	C3-C2	-7.65	1.20	1.51
3	D	806	GOL	O1-C1	4.53	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	805	GOL	O1-C1	4.50	1.61	1.42
3	D	806	GOL	O2-C2	-3.61	1.32	1.43
3	C	805	GOL	O2-C2	-3.15	1.34	1.43
3	D	806	GOL	O3-C3	3.00	1.55	1.42
3	C	805	GOL	C1-C2	-2.96	1.39	1.51
3	C	805	GOL	O3-C3	2.85	1.54	1.42
3	D	806	GOL	C1-C2	-2.77	1.40	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	805	GOL	O3-C3-C2	10.62	161.11	110.20
3	D	806	GOL	O3-C3-C2	10.39	160.03	110.20
3	D	806	GOL	O2-C2-C3	6.60	138.21	109.12
3	C	805	GOL	O2-C2-C3	6.50	137.76	109.12
3	C	805	GOL	O1-C1-C2	3.10	125.09	110.20
3	D	806	GOL	O1-C1-C2	3.07	124.92	110.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	805	GOL	O1-C1-C2-C3
3	C	805	GOL	C1-C2-C3-O3
3	D	806	GOL	C1-C2-C3-O3
3	D	806	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	806	GOL	1	0
3	C	805	GOL	2	0

## 5.7 Other polymers [i](#)

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	267/271 (98%)	0.04	7 (2%) 56 54	10, 18, 35, 47	0
1	B	267/271 (98%)	0.40	20 (7%) 14 13	11, 23, 60, 75	0
1	C	267/271 (98%)	0.21	6 (2%) 62 60	10, 24, 40, 48	0
1	D	267/271 (98%)	0.26	15 (5%) 24 23	11, 24, 46, 58	0
All	All	1068/1084 (98%)	0.23	48 (4%) 33 32	10, 22, 44, 75	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LEU	7.3
1	A	160	LEU	6.7
1	B	153	LEU	5.9
1	D	180	PHE	5.3
1	B	163	ASP	5.2
1	B	159	PRO	4.9
1	D	102	LEU	4.6
1	A	270	ASN	4.4
1	D	160	LEU	4.1
1	B	152	ASN	4.0
1	B	101	GLN	3.7
1	D	101	GLN	3.5
1	D	163	ASP	3.5
1	B	162	ILE	3.5
1	C	20	THR	3.2
1	B	158	ILE	3.2
1	D	140	GLN	3.2
1	D	204	ASP	3.1
1	A	161	VAL	3.0
1	B	180	PHE	3.0
1	B	270	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	165	LEU	2.9
1	C	270	ASN	2.9
1	B	100	LYS	2.7
1	D	86	ARG	2.7
1	B	154	PRO	2.7
1	D	153	LEU	2.6
1	A	75	HIS	2.6
1	B	182	PHE	2.6
1	D	154	PRO	2.6
1	B	166	HIS	2.5
1	B	155	ASP	2.5
1	C	140	GLN	2.5
1	A	170	ASP	2.4
1	A	141	GLU	2.4
1	B	244	ARG	2.4
1	A	159	PRO	2.3
1	D	100	LYS	2.3
1	D	270	ASN	2.3
1	B	75	HIS	2.2
1	B	97	LEU	2.2
1	B	137	LYS	2.1
1	C	139	TYR	2.1
1	C	86	ARG	2.1
1	D	137	LYS	2.1
1	D	139	TYR	2.1
1	D	138	ASP	2.0
1	C	23	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	BFD	B	9	12/13	0.95	0.11	13,15,16,16	0
1	BFD	C	9	12/13	0.95	0.10	14,16,18,19	0
1	BFD	A	9	12/13	0.96	0.11	9,11,12,12	0
1	BFD	D	9	12/13	0.97	0.09	11,13,15,16	0



### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	GOL	C	805	6/6	0.82	0.21	23,29,32,32	0
3	GOL	D	806	6/6	0.83	0.28	32,38,41,41	0
2	MG	C	803	1/1	0.93	0.09	22,22,22,22	0
2	MG	B	802	1/1	0.98	0.08	11,11,11,11	0
2	MG	A	801	1/1	0.98	0.08	11,11,11,11	0
2	MG	D	804	1/1	0.99	0.07	12,12,12,12	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.