



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:02 PM EDT

PDB ID : 4Y0H  
Title : Gamma-aminobutyric acid aminotransferase inactivated by (1S,3S)-3-amino-4-difluoromethylenyl-1-cyclopentanoic acid (CPP-115)  
Authors : Rui, W.; Ruslan, S.; Hyunbeom, L.; Emma, H.D.; Jose, I.J.; Neil, K.; Richard, B.S.; Dali, L.  
Deposited on : 2015-02-06  
Resolution : 1.63 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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	:	2.37.1
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)	:	2.37.1

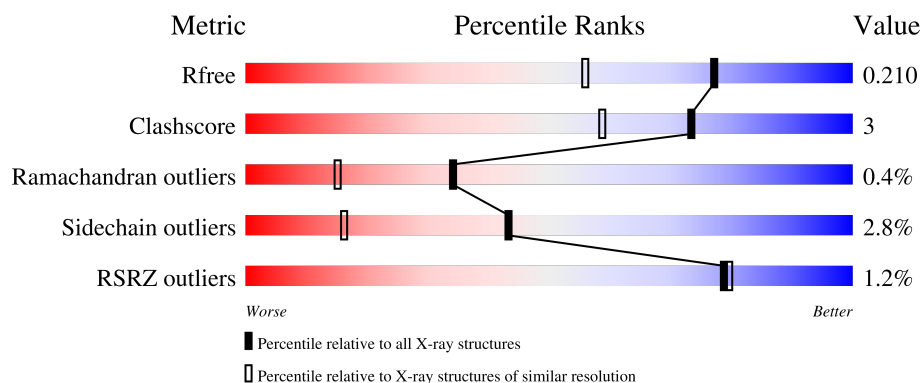
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	463	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">%</span> </div> <div style="width: 88%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">88%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">10%</span> </div> </div>
1	B	463	<div> <div style="width: 2%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">2%</span> </div> <div style="width: 90%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">90%</span> </div> <div style="width: 8%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">8%</span> </div> </div>
1	C	463	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">%</span> </div> <div style="width: 90%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">90%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">10%</span> </div> </div>
1	D	463	<div> <div style="width: 2%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">2%</span> </div> <div style="width: 92%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">92%</span> </div> <div style="width: 8%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">8%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15894 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 4-aminobutyrate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	14	0
			3739	2387	646	681	25			
1	B	462	Total	C	N	O	S	0	12	0
			3742	2382	649	686	25			
1	C	462	Total	C	N	O	S	0	10	0
			3724	2375	644	680	25			
1	D	463	Total	C	N	O	S	0	16	0
			3768	2407	648	687	26			

There are 8 discrepancies between the modelled and reference sequences:

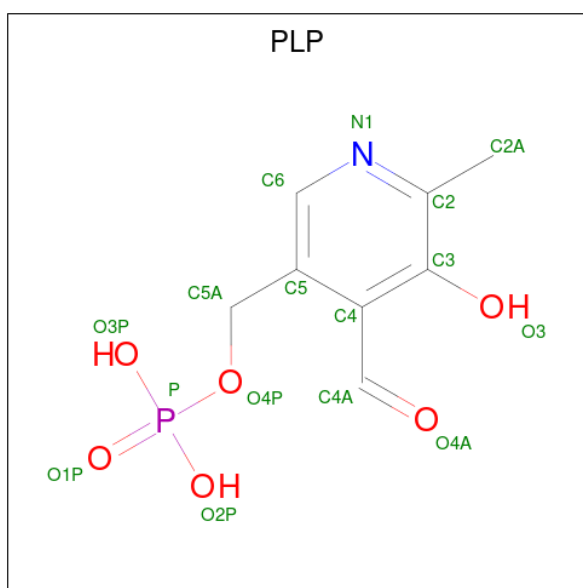
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP P80147
A	158	GLU	GLN	conflict	UNP P80147
B	10	GLY	-	expression tag	UNP P80147
B	158	GLU	GLN	conflict	UNP P80147
C	10	GLY	-	expression tag	UNP P80147
C	158	GLU	GLN	conflict	UNP P80147
D	10	GLY	-	expression tag	UNP P80147
D	158	GLU	GLN	conflict	UNP P80147

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



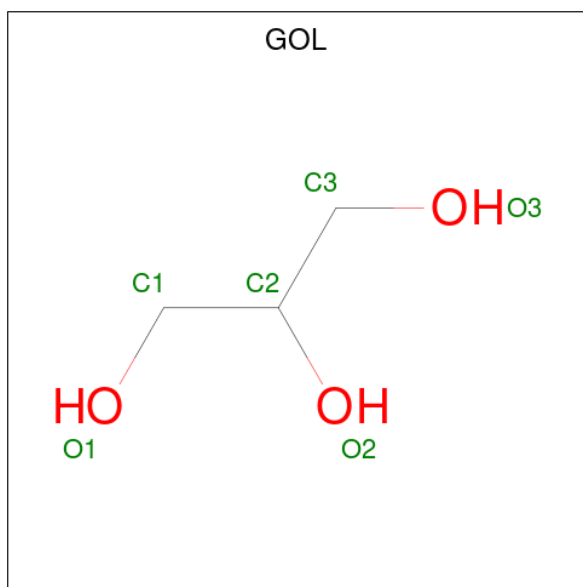
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

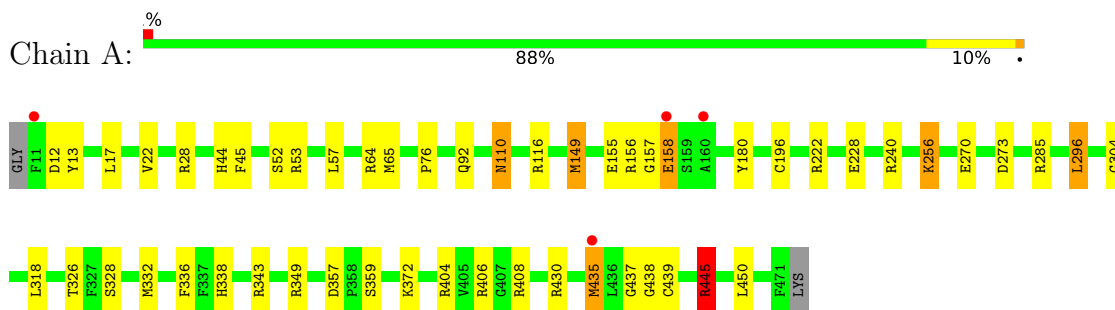
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total	O	0	0
			213	213		
5	B	159	Total	O	0	0
			159	159		
5	C	199	Total	O	0	0
			199	199		
5	D	270	Total	O	0	0
			270	270		

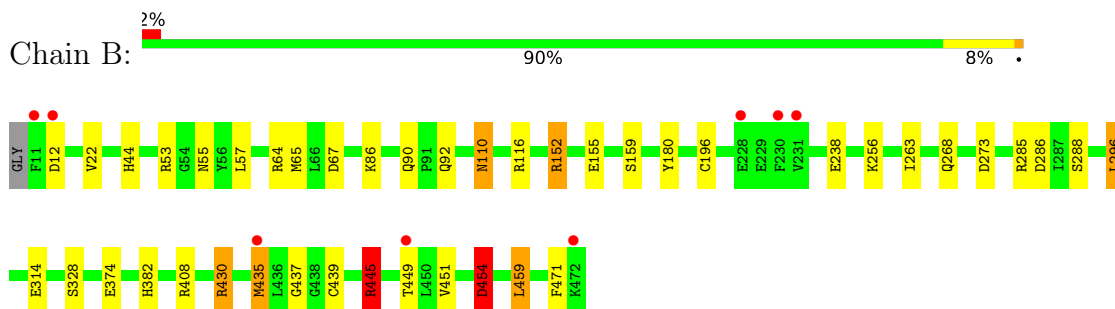
### 3 Residue-property plots [i](#)

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.

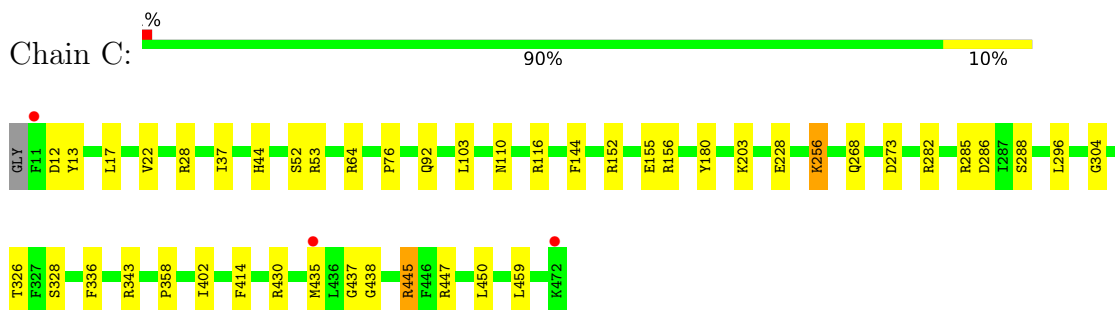
- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial

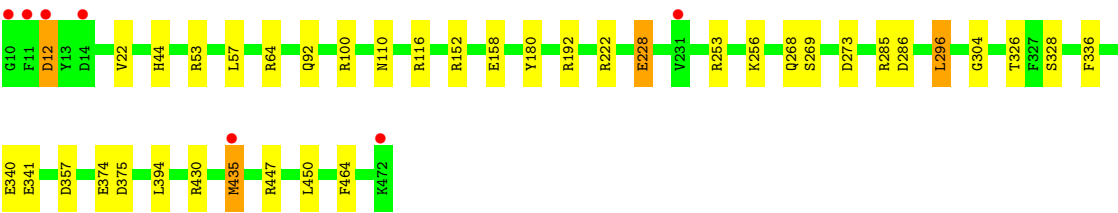


- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.50Å 226.92Å 71.44Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	53.96 – 1.63 36.10 – 1.63	Depositor EDS
% Data completeness (in resolution range)	96.8 (53.96-1.63) 96.8 (36.10-1.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0073, PHENIX	Depositor
R, $R_{free}$	0.176 , 0.203 0.186 , 0.210	Depositor DCC
$R_{free}$ test set	12646 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.01	2/3858 (0.1%)	1.11	23/5205 (0.4%)
1	B	1.02	3/3837 (0.1%)	1.11	17/5183 (0.3%)
1	C	1.05	0/3819	1.12	19/5158 (0.4%)
1	D	1.08	2/3878 (0.1%)	1.08	15/5234 (0.3%)
All	All	1.04	7/15392 (0.0%)	1.10	74/20780 (0.4%)

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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	374	GLU	CD-OE1	-6.25	1.18	1.25
1	A	359	SER	CB-OG	-5.72	1.34	1.42
1	B	12	ASP	CB-CG	5.67	1.63	1.51
1	D	341	GLU	CD-OE1	5.41	1.31	1.25
1	A	196	CYS	CB-SG	-5.22	1.73	1.81
1	B	454	ASP	CB-CG	-5.01	1.41	1.51
1	B	196	CYS	CB-SG	-5.00	1.73	1.81

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	ARG	NE-CZ-NH2	18.38	129.49	120.30
1	A	445	ARG	NE-CZ-NH2	17.79	129.19	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ARG	NE-CZ-NH1	-16.70	111.95	120.30
1	B	445	ARG	NE-CZ-NH2	14.61	127.60	120.30
1	B	445	ARG	NE-CZ-NH1	-13.85	113.38	120.30
1	C	445	ARG	NE-CZ-NH1	-13.62	113.49	120.30
1	D	64	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	A	64	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	B	12	ASP	CB-CG-OD1	9.05	126.44	118.30
1	C	296	LEU	CB-CG-CD2	8.98	126.26	111.00
1	A	28	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	B	64	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	C	343	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	A	404	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	152[A]	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	B	152[B]	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	A	12	ASP	CB-CG-OD1	8.06	125.55	118.30
1	D	64	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	D	447	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	D	192	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	D	447	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	C	447	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	A	408	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	64	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	447	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	D	222	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	445	ARG	CD-NE-CZ	7.06	133.48	123.60
1	D	12	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	64	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	296	LEU	CB-CG-CD2	6.95	122.81	111.00
1	C	64	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	408	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	D	12	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	445	ARG	CD-NE-CZ	6.60	132.83	123.60
1	A	406	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	445	ARG	CD-NE-CZ	6.49	132.68	123.60
1	B	12	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	343	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	28	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	D	286	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	406	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	282	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	D	253	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	28	ARG	NE-CZ-NH2	6.05	123.33	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	D	375	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	116	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	430	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	116	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	100	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	152[A]	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	B	152[B]	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	A	149	MET	CG-SD-CE	-5.62	91.20	100.20
1	C	12	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	156	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	296	LEU	CB-CG-CD2	5.55	120.43	111.00
1	A	222	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	156	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	144	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	A	240	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	116	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	286	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	286	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	116	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	357	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	64	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	445	ARG	CB-CG-CD	5.15	125.00	111.60
1	A	318	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	C	445	ARG	CB-CG-CD	5.11	124.89	111.60
1	D	357	ASP	CB-CG-OD1	5.11	122.89	118.30
1	C	343	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	408	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	144	PHE	CB-CG-CD1	5.02	124.32	120.80
1	B	459	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	PHE	Peptide

## 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	3739	0	3713	31	0
1	B	3742	0	3655	29	0
1	C	3724	0	3654	22	0
1	D	3768	0	3695	17	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
3	C	15	0	6	0	0
3	D	15	0	6	0	0
4	B	6	0	7	3	0
4	C	6	0	8	0	0
5	A	213	0	0	4	0
5	B	159	0	0	1	0
5	C	199	0	0	3	0
5	D	270	0	0	3	0
All	All	15894	0	14756	99	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 3.

All (99) 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:53[B]:ARG:HG3	1:A:53[B]:ARG:HH11	1.12	1.05
1:D:53[B]:ARG:HG2	1:D:53[B]:ARG:HH11	1.12	1.03
1:D:228:GLU:HG3	5:D:696:HOH:O	1.59	1.01
1:B:65:MET:HB2	1:B:435[B]:MET:HE2	1.47	0.96
1:A:155:GLU:OE1	1:A:180:TYR:OH	1.87	0.91
1:D:53[B]:ARG:HH11	1:D:53[B]:ARG:CG	1.84	0.90
1:C:152:ARG:HD2	1:C:180:TYR:OH	1.72	0.90
1:A:65:MET:HB2	1:A:435[B]:MET:HE3	1.57	0.84
1:D:53[B]:ARG:HG2	1:D:53[B]:ARG:NH1	1.92	0.81
1:B:65:MET:HB2	1:B:435[B]:MET:CE	2.12	0.80
1:A:157:GLY:HA3	1:A:158:GLU:HB2	1.67	0.76
1:B:57:LEU:HB3	1:B:435[B]:MET:HE1	1.72	0.71
1:B:155:GLU:OE1	1:B:180:TYR:OH	2.08	0.71
1:C:17:LEU:HB3	5:C:797:HOH:O	1.91	0.70
1:A:53[B]:ARG:HG3	1:A:53[B]:ARG:NH1	1.93	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53[B]:ARG:HG2	1:C:53[B]:ARG:HH11	1.56	0.70
1:C:155:GLU:OE1	1:C:180:TYR:OH	2.10	0.69
1:A:57:LEU:HD23	1:A:435[B]:MET:HE1	1.73	0.68
1:B:449[A]:THR:HG23	1:B:451:VAL:H	1.58	0.68
1:B:314:GLU:HA	4:B:501:GOL:H12	1.74	0.68
1:A:65:MET:SD	1:A:435[B]:MET:HE2	2.35	0.67
1:B:314:GLU:HA	4:B:501:GOL:C1	2.25	0.67
1:B:152[B]:ARG:HH21	1:B:155:GLU:HB2	1.59	0.66
1:D:53[B]:ARG:CG	1:D:53[B]:ARG:NH1	2.50	0.66
1:B:152[B]:ARG:HE	1:B:152[B]:ARG:HA	1.60	0.65
1:B:437:GLY:N	5:B:666:HOH:O	2.25	0.64
1:D:152:ARG:HG2	1:D:180[B]:TYR:HE2	1.64	0.63
1:C:268:GLN:O	1:C:273:ASP:HA	1.99	0.62
1:A:437:GLY:N	5:A:744:HOH:O	2.31	0.61
1:C:53[B]:ARG:HG2	1:C:53[B]:ARG:NH1	2.17	0.59
1:B:263:ILE:HD12	1:B:296:LEU:HD13	1.85	0.58
1:A:65:MET:HB2	1:A:435[B]:MET:CE	2.30	0.57
1:C:152:ARG:HD2	1:C:180:TYR:CZ	2.39	0.57
1:A:52:SER:O	1:A:53[B]:ARG:NH1	2.38	0.57
1:B:382:HIS:NE2	1:B:454:ASP:OD2	2.38	0.55
1:A:53[B]:ARG:HH11	1:A:53[B]:ARG:CG	2.00	0.54
1:B:57:LEU:HB3	1:B:435[B]:MET:CE	2.38	0.53
1:B:152[B]:ARG:HH21	1:B:155:GLU:CB	2.20	0.53
1:B:55:ASN:ND2	1:B:449[A]:THR:HG22	2.25	0.52
1:D:12:ASP:OD2	5:D:633:HOH:O	2.19	0.51
1:D:152:ARG:HG2	1:D:180[B]:TYR:CE2	2.43	0.51
1:B:92[B]:GLN:H	1:B:92[B]:GLN:CD	2.14	0.51
1:A:157:GLY:CA	1:A:158:GLU:HB2	2.39	0.51
1:A:439:CYS:HB3	1:A:445:ARG:HD2	1.93	0.50
1:B:268:GLN:O	1:B:273:ASP:HA	2.11	0.50
1:D:57:LEU:HD23	1:D:435[B]:MET:HE1	1.94	0.50
1:A:65:MET:CE	1:A:435[B]:MET:HE2	2.42	0.50
1:C:13:TYR:CE2	1:C:53[B]:ARG:HG3	2.48	0.49
1:B:152[B]:ARG:HE	1:B:152[B]:ARG:CA	2.24	0.49
1:A:326:THR:HG22	1:A:336:PHE:HB3	1.95	0.49
1:D:268:GLN:O	1:D:273:ASP:HA	2.13	0.49
1:A:438:GLY:O	1:A:445:ARG:HD3	2.12	0.49
1:A:57:LEU:HB3	1:A:435[B]:MET:CE	2.42	0.48
1:C:37[B]:ILE:O	1:C:37[B]:ILE:HG22	2.14	0.48
1:C:437:GLY:N	5:C:744:HOH:O	2.36	0.48
1:B:65:MET:CB	1:B:435[B]:MET:CE	2.89	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:HA	1:B:435[A]:MET:HB2	1.97	0.46
1:C:22:VAL:CG1	1:C:430:ARG:HD3	2.45	0.46
1:A:256:LYS:N	1:A:256:LYS:HD3	2.30	0.46
1:D:152:ARG:HD2	1:D:180[B]:TYR:OH	2.16	0.46
1:A:13:TYR:CE2	1:A:53[A]:ARG:HB2	2.51	0.46
1:B:110:ASN:HD22	1:B:110:ASN:C	2.18	0.46
1:C:52:SER:C	1:C:53[B]:ARG:HG2	2.36	0.46
1:C:326:THR:HG22	1:C:336:PHE:HB3	1.98	0.46
1:B:110:ASN:C	1:B:110:ASN:ND2	2.68	0.45
1:D:326:THR:HG22	1:D:336:PHE:HB3	1.98	0.45
1:A:338:HIS:HE1	5:A:627:HOH:O	1.99	0.45
1:B:86:LYS:O	1:B:90[A]:GLN:HG2	2.16	0.45
1:D:435[B]:MET:HB3	1:D:435[B]:MET:HE3	1.64	0.45
1:A:22:VAL:HG11	1:A:430:ARG:HD3	2.00	0.44
1:A:45:PHE:HZ	1:A:435[B]:MET:CE	2.30	0.44
1:B:152[A]:ARG:HH11	1:B:152[A]:ARG:HD2	1.60	0.44
1:A:149:MET:HG2	1:A:349:ARG:NH2	2.32	0.44
1:A:338:HIS:CE1	5:A:627:HOH:O	2.69	0.44
1:A:304:GLY:O	1:A:450:LEU:HD11	2.18	0.44
1:B:314:GLU:HA	4:B:501:GOL:H11	1.99	0.44
1:D:304:GLY:O	1:D:450:LEU:HD11	2.17	0.44
1:A:332[B]:MET:HE2	1:A:332[B]:MET:HB3	1.85	0.44
1:C:304:GLY:O	1:C:450:LEU:HD11	2.19	0.43
1:A:110:ASN:C	1:A:110:ASN:HD22	2.21	0.43
1:C:103:LEU:HD21	1:C:358:PRO:HG3	2.00	0.43
1:C:438:GLY:O	1:C:445:ARG:HD3	2.19	0.43
1:D:22:VAL:HG11	1:D:430:ARG:HD3	2.00	0.42
1:A:57:LEU:HB3	1:A:435[B]:MET:HE3	2.01	0.42
1:C:402[A]:ILE:HD12	1:C:414:PHE:CE1	2.54	0.42
1:A:372:LYS:NZ	5:A:617:HOH:O	2.51	0.42
1:B:67:ASP:HB2	1:B:435[B]:MET:HE1	2.02	0.42
1:C:52:SER:O	1:C:53[B]:ARG:HG2	2.18	0.42
1:B:22:VAL:CG1	1:B:430:ARG:HD3	2.49	0.42
1:C:53[B]:ARG:HH11	1:C:53[B]:ARG:CG	2.28	0.42
1:A:270[B]:GLU:O	1:A:270[B]:GLU:HG3	2.19	0.41
1:D:394:LEU:HD13	1:D:464[B]:PHE:CD2	2.55	0.41
1:C:256:LYS:HE3	1:C:256:LYS:HB2	1.87	0.41
1:D:269:SER:HB2	5:D:810:HOH:O	2.19	0.41
1:C:430:ARG:HD2	5:C:759:HOH:O	2.21	0.41
1:A:110:ASN:C	1:A:110:ASN:ND2	2.73	0.41
1:B:57:LEU:HD23	1:B:435[B]:MET:SD	2.61	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:CYS:HB3	1:B:445:ARG:HD2	2.03	0.41
1:C:37[B]:ILE:O	1:C:37[B]:ILE:CG2	2.69	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	473/463 (102%)	453 (96%)	17 (4%)	3 (1%)	25	8
1	B	472/463 (102%)	455 (96%)	16 (3%)	1 (0%)	47	26
1	C	470/463 (102%)	454 (97%)	14 (3%)	2 (0%)	34	15
1	D	477/463 (103%)	461 (97%)	15 (3%)	1 (0%)	47	26
All	All	1892/1852 (102%)	1823 (96%)	62 (3%)	7 (0%)	34	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	GLU
1	A	328	SER
1	B	328	SER
1	D	328	SER
1	C	328	SER
1	A	76	PRO
1	C	76	PRO

### 5.3.2 Protein sidechains [i](#)

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	410/401 (102%)	398 (97%)	12 (3%)	42	15
1	B	403/401 (100%)	388 (96%)	15 (4%)	34	9
1	C	402/401 (100%)	390 (97%)	12 (3%)	41	14
1	D	406/401 (101%)	395 (97%)	11 (3%)	44	18
All	All	1621/1604 (101%)	1571 (97%)	50 (3%)	43	13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	44	HIS
1	A	92	GLN
1	A	110	ASN
1	A	228	GLU
1	A	256	LYS
1	A	273	ASP
1	A	285	ARG
1	A	296	LEU
1	A	435[A]	MET
1	A	435[B]	MET
1	A	445	ARG
1	B	44	HIS
1	B	53[A]	ARG
1	B	53[B]	ARG
1	B	110	ASN
1	B	159	SER
1	B	256	LYS
1	B	285	ARG
1	B	288	SER
1	B	296	LEU
1	B	374	GLU
1	B	435[A]	MET
1	B	435[B]	MET
1	B	445	ARG
1	B	454	ASP
1	B	459	LEU
1	C	44	HIS
1	C	92	GLN
1	C	110	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	203	LYS
1	C	228[A]	GLU
1	C	228[B]	GLU
1	C	256	LYS
1	C	285	ARG
1	C	288	SER
1	C	435[A]	MET
1	C	435[B]	MET
1	C	459	LEU
1	D	44	HIS
1	D	92	GLN
1	D	110	ASN
1	D	158	GLU
1	D	228	GLU
1	D	256	LYS
1	D	285	ARG
1	D	296	LEU
1	D	340	GLU
1	D	435[A]	MET
1	D	435[B]	MET

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

Mol	Chain	Res	Type
1	A	44	HIS
1	A	110	ASN
1	A	338	HIS
1	B	55	ASN
1	B	110	ASN
1	B	338	HIS
1	C	44	HIS
1	C	55	ASN
1	C	110	ASN
1	C	338	HIS
1	D	55	ASN
1	D	110	ASN
1	D	338	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands 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$
2	FES	C	501	1	0,4,4	-	-	-		
3	PLP	C	503	1	15,15,16	2.92	4 (26%)	20,22,23	1.72	6 (30%)
3	PLP	B	502	1	15,15,16	3.00	5 (33%)	20,22,23	1.44	3 (15%)
2	FES	A	501	1	0,4,4	-	-	-		
3	PLP	D	501	1	15,15,16	2.12	4 (26%)	20,22,23	2.14	6 (30%)
4	GOL	C	502	-	5,5,5	0.64	0	5,5,5	1.09	0
4	GOL	B	501	-	5,5,5	1.06	1 (20%)	5,5,5	1.60	2 (40%)
3	PLP	A	502	1	15,15,16	2.25	4 (26%)	20,22,23	2.15	7 (35%)

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	FES	C	501	1	-	-	0/1/1/1
3	PLP	C	503	1	-	0/6/6/8	0/1/1/1
3	PLP	B	502	1	-	0/6/6/8	0/1/1/1
3	PLP	D	501	1	-	0/6/6/8	0/1/1/1
4	GOL	C	502	-	-	2/4/4/4	-
2	FES	A	501	1	-	-	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	501	-	-	1/4/4/4	-
3	PLP	A	502	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	PLP	C3-C2	8.74	1.49	1.40
3	B	502	PLP	C5-C4	7.51	1.48	1.40
3	B	502	PLP	C3-C2	6.81	1.47	1.40
3	D	501	PLP	C3-C2	5.97	1.46	1.40
3	A	502	PLP	C5-C4	5.56	1.46	1.40
3	C	503	PLP	C5-C4	4.84	1.45	1.40
3	C	503	PLP	C3-C4	3.95	1.48	1.40
3	A	502	PLP	C3-C2	3.78	1.44	1.40
3	B	502	PLP	P-O4P	3.43	1.71	1.60
3	B	502	PLP	C3-C4	3.02	1.46	1.40
3	D	501	PLP	C5-C4	2.61	1.43	1.40
3	D	501	PLP	C3-C4	2.44	1.45	1.40
3	D	501	PLP	C2A-C2	-2.33	1.46	1.50
4	B	501	GOL	O2-C2	-2.27	1.36	1.43
3	A	502	PLP	C6-N1	2.24	1.39	1.34
3	B	502	PLP	C6-N1	2.20	1.39	1.34
3	C	503	PLP	O3-C3	-2.04	1.32	1.37
3	A	502	PLP	C2A-C2	-2.04	1.46	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	PLP	C4A-C4-C5	5.76	126.87	120.94
3	A	502	PLP	C6-C5-C4	5.58	122.55	118.16
3	D	501	PLP	O4P-C5A-C5	4.46	117.84	109.35
3	A	502	PLP	O3P-P-O2P	3.64	121.55	107.64
3	A	502	PLP	O4P-C5A-C5	3.19	115.43	109.35
3	A	502	PLP	C4A-C4-C5	3.17	124.20	120.94
3	A	502	PLP	C3-C4-C5	-3.17	115.32	118.74
3	C	503	PLP	C6-C5-C4	3.15	120.64	118.16
3	C	503	PLP	C6-N1-C2	3.07	124.85	119.17
3	B	502	PLP	O3P-P-O4P	-3.01	98.72	106.73
3	D	501	PLP	O3P-P-O2P	2.92	118.81	107.64
3	C	503	PLP	C2A-C2-N1	2.38	122.32	117.67
3	C	503	PLP	C4-C3-C2	-2.34	116.61	120.07
3	B	502	PLP	C6-N1-C2	2.32	123.47	119.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	PLP	C4A-C4-C3	-2.32	116.57	120.50
3	D	501	PLP	C2A-C2-N1	2.30	122.16	117.67
3	C	503	PLP	O3-C3-C2	2.23	122.34	117.49
3	B	502	PLP	O4P-P-O1P	-2.21	100.29	106.47
3	D	501	PLP	C3-C4-C5	-2.18	116.39	118.74
3	C	503	PLP	O4P-P-O1P	-2.14	100.46	106.47
4	B	501	GOL	O2-C2-C3	-2.13	99.75	109.12
4	B	501	GOL	C3-C2-C1	2.05	119.69	111.70
3	A	502	PLP	O3P-P-O4P	-2.03	101.34	106.73
3	A	502	PLP	O3-C3-C4	2.02	123.43	118.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	GOL	3	0

## 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	461/463 (99%)	-0.25	4 (0%) 84 85	10, 17, 33, 65	0
1	B	462/463 (99%)	-0.15	8 (1%) 70 71	12, 19, 33, 86	1 (0%)
1	C	462/463 (99%)	-0.22	3 (0%) 89 89	9, 18, 31, 51	0
1	D	463/463 (100%)	-0.25	7 (1%) 73 74	9, 15, 28, 84	0
All	All	1848/1852 (99%)	-0.22	22 (1%) 79 79	9, 17, 32, 86	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PHE	10.0
1	D	10	GLY	8.0
1	D	11	PHE	7.1
1	A	158	GLU	4.9
1	B	472	LYS	4.2
1	C	11	PHE	3.6
1	A	11	PHE	3.5
1	B	231	VAL	3.0
1	D	14	ASP	2.9
1	B	12	ASP	2.8
1	D	12	ASP	2.8
1	C	472	LYS	2.7
1	D	435[A]	MET	2.6
1	D	472	LYS	2.5
1	B	228	GLU	2.5
1	B	230	PHE	2.4
1	D	231	VAL	2.3
1	B	435[A]	MET	2.3
1	A	435[A]	MET	2.2
1	A	160	ALA	2.2
1	B	449[A]	THR	2.1
1	C	435[A]	MET	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 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
4	GOL	C	502	6/6	0.87	0.14	36,47,48,48	0
4	GOL	B	501	6/6	0.89	0.28	23,38,46,49	0
3	PLP	B	502	15/16	0.97	0.10	13,16,19,22	0
3	PLP	D	501	15/16	0.98	0.11	10,14,17,24	0
3	PLP	A	502	15/16	0.98	0.09	12,15,19,20	0
3	PLP	C	503	15/16	0.98	0.09	10,12,15,21	0
2	FES	A	501	4/4	0.99	0.07	13,13,13,13	0
2	FES	C	501	4/4	1.00	0.07	11,11,11,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.