



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:49 AM UTC

PDB ID : 4Y0H / pdb_00004y0h
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

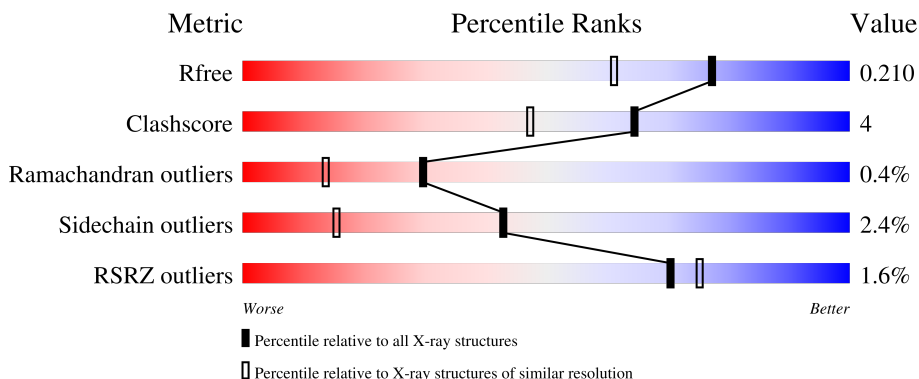
1 Overall quality at a glance

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}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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 ≥ 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	2% 91% 7% .
1	B	463	% 89% 10% .
1	C	463	2% 90% 8% .
1	D	463	2% 92% 8% .

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:

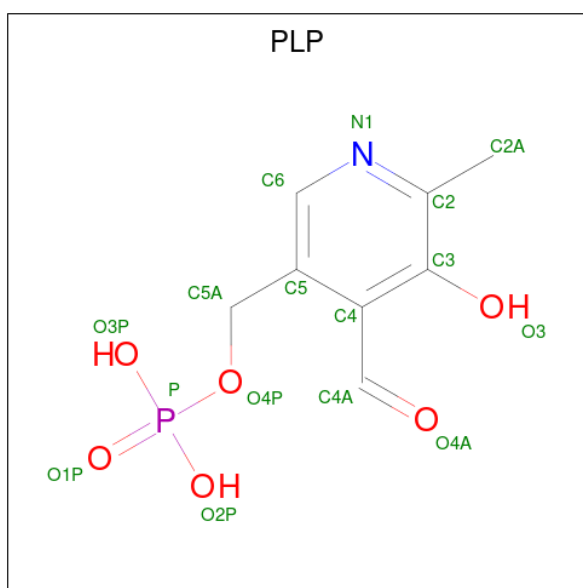
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP P80147
A	158	GLU	GLN	conflict	UNP P80147
B	10	GLY	-	expression tag	UNP P80147
B	158	GLU	GLN	conflict	UNP P80147
C	10	GLY	-	expression tag	UNP P80147
C	158	GLU	GLN	conflict	UNP P80147
D	10	GLY	-	expression tag	UNP P80147
D	158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

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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 (CCD ID: 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 (CCD ID: 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		

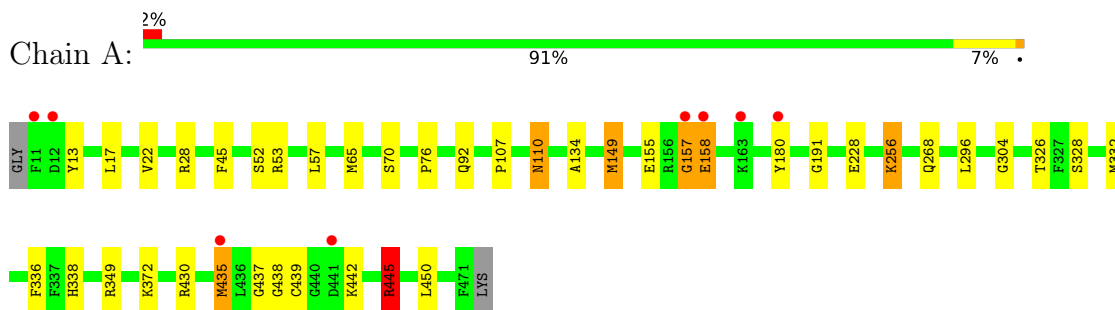
- Molecule 5 is water.

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		

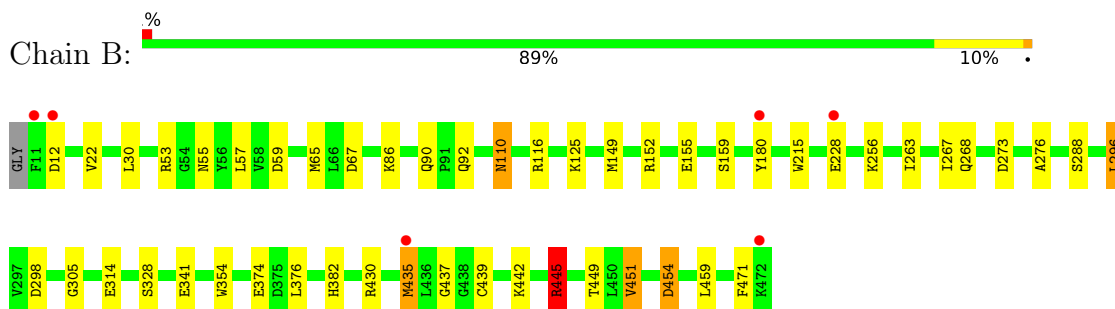
3 Residue-property plots [i](#)

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.

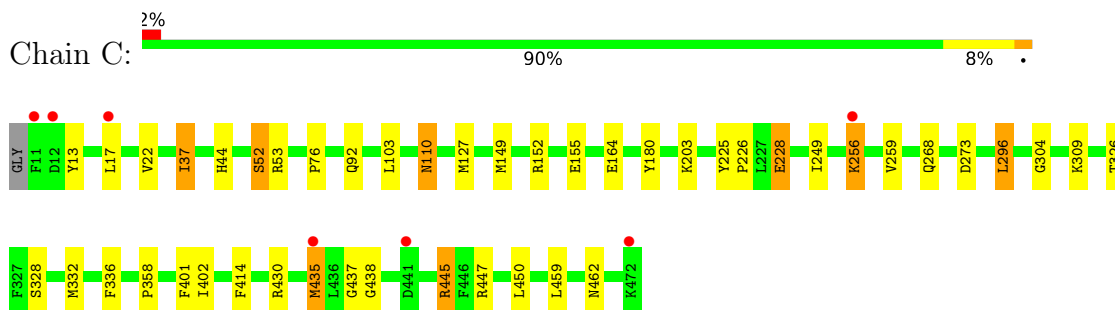
- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial

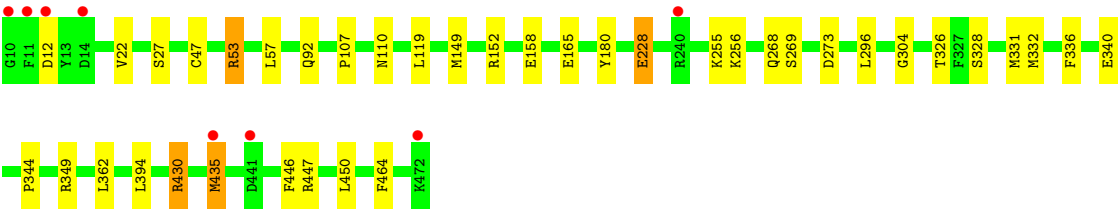


- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



- 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, α , β , γ	69.50Å 226.92Å 71.44Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	53.96 – 1.63 53.96 – 1.63	Depositor EDS
% Data completeness (in resolution range)	96.8 (53.96-1.63) 96.9 (53.96-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, PLP, FES

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	1.27	6/3858 (0.2%)	1.17	8/5205 (0.2%)
1	B	1.33	9/3837 (0.2%)	1.20	11/5183 (0.2%)
1	C	1.35	7/3819 (0.2%)	1.25	10/5158 (0.2%)
1	D	1.34	7/3878 (0.2%)	1.18	4/5234 (0.1%)
All	All	1.32	29/15392 (0.2%)	1.20	33/20780 (0.2%)

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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	MET	SD-CE	-8.74	1.57	1.79
1	B	149	MET	SD-CE	-7.86	1.59	1.79
1	D	107	PRO	CA-CB	-7.34	1.47	1.54
1	B	298	ASP	N-CA	7.19	1.55	1.46
1	B	12	ASP	CA-C	7.18	1.61	1.52
1	C	149	MET	SD-CE	-6.76	1.62	1.79
1	A	107	PRO	CA-CB	-6.43	1.48	1.54
1	C	164	GLU	CA-C	6.40	1.61	1.52
1	C	259	VAL	C-O	6.26	1.29	1.23
1	A	442	LYS	C-O	-6.11	1.18	1.24
1	A	70	SER	CA-C	6.01	1.60	1.53
1	B	30	LEU	N-CA	5.95	1.53	1.46
1	A	268	GLN	N-CA	5.82	1.53	1.46
1	D	165	GLU	N-CA	5.81	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	446	PHE	CA-C	-5.67	1.45	1.52
1	B	341	GLU	C-O	-5.49	1.17	1.24
1	C	52	SER	C-O	5.41	1.30	1.23
1	B	354	TRP	CA-C	5.39	1.59	1.52
1	A	149	MET	SD-CE	-5.33	1.66	1.79
1	A	191	GLY	C-O	5.27	1.28	1.23
1	D	430	ARG	CA-C	5.25	1.59	1.52
1	B	116	ARG	N-CA	5.25	1.52	1.46
1	C	249	ILE	CA-CB	-5.24	1.48	1.54
1	B	276	ALA	C-O	-5.20	1.17	1.23
1	D	27	SER	N-CA	5.19	1.52	1.46
1	C	445	ARG	CD-NE	-5.19	1.39	1.46
1	B	125	LYS	CA-C	-5.10	1.46	1.52
1	D	362	LEU	N-CA	5.04	1.52	1.46
1	D	255	LYS	C-O	-5.01	1.16	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	ARG	NE-CZ-NH2	11.43	129.49	119.20
1	A	445	ARG	NE-CZ-NH2	11.10	129.19	119.20
1	A	445	ARG	NE-CZ-NH1	-9.55	111.95	121.50
1	B	445	ARG	NE-CZ-NH2	9.34	127.60	119.20
1	B	445	ARG	NE-CZ-NH1	-8.12	113.38	121.50
1	C	445	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	B	376	LEU	N-CA-C	6.87	121.25	113.01
1	A	445	ARG	CD-NE-CZ	6.49	133.48	124.40
1	A	157	GLY	CA-C-N	6.35	133.12	121.70
1	A	157	GLY	C-N-CA	6.35	133.12	121.70
1	B	305	GLY	N-CA-C	6.06	122.00	114.37
1	C	445	ARG	CD-NE-CZ	6.02	132.83	124.40
1	A	28	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	A	445	ARG	CB-CG-CD	5.95	125.00	111.30
1	C	37[A]	ILE	N-CA-C	-5.93	106.96	113.43
1	C	37[B]	ILE	N-CA-C	-5.93	106.96	113.43
1	D	119	LEU	N-CA-C	5.93	117.74	111.28
1	B	445	ARG	CD-NE-CZ	5.92	132.68	124.40
1	C	445	ARG	CB-CG-CD	5.91	124.89	111.30
1	C	309	LYS	N-CA-C	-5.51	100.98	109.52
1	C	462	ASN	N-CA-C	5.46	116.91	111.07
1	D	447	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	C	447	ARG	NE-CZ-NH2	5.41	124.07	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ARG	CB-CG-CD	5.20	123.25	111.30
1	C	296	LEU	CB-CG-CD2	5.19	126.26	110.70
1	B	442	LYS	N-CA-C	5.17	118.81	112.03
1	B	267	ILE	N-CA-C	-5.12	100.69	108.17
1	B	215	TRP	CA-C-N	-5.10	114.73	120.14
1	B	215	TRP	C-N-CA	-5.10	114.73	120.14
1	D	447	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	134	ALA	N-CA-C	5.04	119.14	112.89
1	B	451	VAL	O-C-N	5.03	126.61	122.09
1	D	47	CYS	N-CA-C	5.02	117.58	109.40

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 [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	3739	0	3713	35	0
1	B	3742	0	3655	28	0
1	C	3724	0	3654	31	0
1	D	3768	0	3695	21	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15894	0	14756	115	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 (115) 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:B:65:MET:HB2	1:B:435[B]:MET:HE2	1.19	1.12
1:A:53[B]:ARG:HG3	1:A:53[B]:ARG:HH11	1.12	1.05
1:A:65:MET:HB2	1:A:435[B]:MET:HE3	1.35	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:57:LEU:HB3	1:B:435[B]:MET:HE1	1.42	0.99
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:B:65:MET:CB	1:B:435[B]:MET:HE2	2.02	0.88
1:D:53[B]:ARG:HG2	1:D:53[B]:ARG:NH1	1.92	0.81
1:A:157:GLY:HA3	1:A:158:GLU:HB2	1.67	0.76
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
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: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: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:A:57:LEU:HB3	1:A:435[B]:MET:HE1	1.79	0.65
1:A:57:LEU:HD23	1:A:435[B]:MET:HE1	1.78	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:D:149[B]:MET:HE1	1:D:349:ARG:HB3	1.85	0.59
1:B:263:ILE:HD12	1:B:296:LEU:HD13	1.85	0.58
1:B:65:MET:HB2	1:B:435[B]:MET:CE	2.12	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:44:HIS:HD2	1:C:435[A]:MET:HE1	1.70	0.56
1:B:92[B]:GLN:H	1:B:92[B]:GLN:CD	2.14	0.55
1:A:45:PHE:HZ	1:A:435[B]:MET:HE2	1.71	0.55
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:A:45:PHE:CZ	1:A:435[B]:MET:HE2	2.43	0.53
1:A:65:MET:CB	1:A:435[B]:MET:HE3	2.23	0.53
1:A:65:MET:HE3	1:A: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:C:44:HIS:CD2	1:C:435[A]:MET:HE1	2.45	0.52
1:B:110:ASN:ND2	1:B:110:ASN:C	2.68	0.51
1:D:57:LEU:HD23	1:D:435[B]:MET:HE1	1.93	0.51
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:A:157:GLY:CA	1:A:158:GLU:HB2	2.39	0.51
1:C:52:SER:C	1:C:53[B]:ARG:HG2	2.36	0.50
1:B:110:ASN:C	1:B:110:ASN:HD22	2.18	0.50
1:A:439:CYS:HB3	1:A:445:ARG:HD2	1.93	0.50
1:C:430:ARG:HE	1:C:435[A]:MET:HE3	1.75	0.50
1:B:268:GLN:O	1:B:273:ASP:HA	2.11	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: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:C:332[B]:MET:HE2	1:C:332[B]:MET:HB3	1.79	0.48
1:A:110:ASN:HD22	1:A:110:ASN:C	2.21	0.48
1:A:57:LEU:HB3	1:A:435[B]:MET:CE	2.42	0.48
1:A:332[B]:MET:HE2	1:A:332[B]:MET:HB3	1.56	0.46
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:149:MET:HB2	1:A:149:MET:HE2	1.72	0.46
1:A:13:TYR:CE2	1:A:53[A]:ARG:HB2	2.51	0.46
1:C:326:THR:HG22	1:C:336:PHE:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:THR:HG22	1:D:336:PHE:HB3	1.98	0.45
1:A:110:ASN:C	1:A:110:ASN:ND2	2.73	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:332[B]:MET:HE2	1:D:332[B]:MET:HB3	1.61	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:C:304:GLY:O	1:C:450:LEU:HD11	2.19	0.43
1:C:103:LEU:HD21	1:C:358:PRO:HG3	2.00	0.43
1:C:401:PHE:C	1:C:402[A]:ILE:HD13	2.43	0.43
1:D:435[B]:MET:HB2	1:D:435[B]:MET:HE2	1.50	0.43
1:A:65:MET:CE	1:A:435[B]:MET:HE2	2.49	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: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:C:52:SER:O	1:C:53[B]:ARG:HG2	2.18	0.42
1:A:65:MET:SD	1:A:435[B]:MET:HE2	2.59	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:C:110:ASN:C	1:C:110:ASN:HD22	2.27	0.42
1:A:57:LEU:HD23	1:A:435[B]:MET:CE	2.49	0.42
1:C:228[A]:GLU:H	1:C:228[A]:GLU:CD	2.28	0.42
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:D:331:MET:C	1:D:332[A]:MET:HG2	2.46	0.41
1:D:149[A]:MET:HE1	1:D:344:PRO:HB3	2.03	0.41
1:C:430:ARG:HD2	5:C:759:HOH:O	2.21	0.41
1:B:57:LEU:HD23	1:B:435[B]:MET:SD	2.61	0.41
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
1:C:225:TYR:HA	1:C:226:PRO:C	2.47	0.40
1:C:110:ASN:C	1:C:110:ASN:ND2	2.80	0.40
1:B:59:ASP:C	1:B:59:ASP:OD1	2.65	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%)	21	7
1	B	472/463 (102%)	455 (96%)	16 (3%)	1 (0%)	43	27
1	C	470/463 (102%)	454 (97%)	14 (3%)	2 (0%)	30	14
1	D	477/463 (103%)	461 (97%)	15 (3%)	1 (0%)	43	27
All	All	1892/1852 (102%)	1823 (96%)	62 (3%)	7 (0%)	30	14

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%)	401 (98%)	9 (2%)	45	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	403/401 (100%)	389 (96%)	14 (4%)	32 6
1	C	402/401 (100%)	392 (98%)	10 (2%)	42 14
1	D	406/401 (101%)	395 (97%)	11 (3%)	39 13
All	All	1621/1604 (101%)	1577 (97%)	44 (3%)	43 13

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	92	GLN
1	A	110	ASN
1	A	228	GLU
1	A	256	LYS
1	A	296	LEU
1	A	435[A]	MET
1	A	435[B]	MET
1	A	445	ARG
1	B	53[A]	ARG
1	B	53[B]	ARG
1	B	110	ASN
1	B	159	SER
1	B	228	GLU
1	B	256	LYS
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	92	GLN
1	C	110	ASN
1	C	203	LYS
1	C	228[A]	GLU
1	C	228[B]	GLU
1	C	256	LYS
1	C	296	LEU
1	C	435[A]	MET
1	C	435[B]	MET
1	C	459	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	53[A]	ARG
1	D	53[B]	ARG
1	D	92	GLN
1	D	110	ASN
1	D	158	GLU
1	D	228	GLU
1	D	256	LYS
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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	110	ASN
1	A	142	ASN
1	A	268	GLN
1	A	274	ASN
1	A	338	HIS
1	A	369	ASN
1	B	38	GLN
1	B	55	ASN
1	B	110	ASN
1	B	142	ASN
1	B	268	GLN
1	B	274	ASN
1	B	315	HIS
1	B	338	HIS
1	B	379	ASN
1	B	455	HIS
1	C	38	GLN
1	C	44	HIS
1	C	110	ASN
1	C	268	GLN
1	C	274	ASN
1	C	338	HIS
1	C	458	HIS
1	D	38	GLN
1	D	110	ASN
1	D	268	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	274	ASN
1	D	338	HIS
1	D	369	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	GOL	B	501	-	5,5,5	1.08	1 (20%)	5,5,5	1.69	2 (40%)
3	PLP	C	503	1	15,15,16	2.88	4 (26%)	21,22,23	1.69	7 (33%)
3	PLP	B	502	1	15,15,16	2.95	5 (33%)	21,22,23	1.41	3 (14%)
4	GOL	C	502	-	5,5,5	0.66	0	5,5,5	1.18	0
2	FES	A	501	1	0,4,4	-	-	-	-	-
2	FES	C	501	1	0,4,4	-	-	-	-	-
3	PLP	A	502	1	15,15,16	2.25	6 (40%)	21,22,23	2.11	8 (38%)
3	PLP	D	501	1	15,15,16	2.11	5 (33%)	21,22,23	2.12	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	501	-	-	1/4/4/4	-
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
4	GOL	C	502	-	-	2/4/4/4	-
2	FES	A	501	1	-	-	0/1/1/1
2	FES	C	501	1	-	-	0/1/1/1
3	PLP	A	502	1	-	0/6/6/8	0/1/1/1
3	PLP	D	501	1	-	0/6/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	PLP	C3-C2	8.36	1.49	1.41
3	B	502	PLP	C5-C4	7.34	1.48	1.40
3	B	502	PLP	C3-C2	6.50	1.47	1.41
3	D	501	PLP	C3-C2	5.69	1.46	1.41
3	A	502	PLP	C5-C4	5.43	1.46	1.40
3	C	503	PLP	C5-C4	4.72	1.45	1.40
3	C	503	PLP	C3-C4	4.31	1.48	1.40
3	A	502	PLP	C3-C2	3.58	1.44	1.41
3	B	502	PLP	P-O4P	3.47	1.71	1.60
3	B	502	PLP	C3-C4	3.29	1.46	1.40
3	D	501	PLP	C3-C4	2.66	1.45	1.40
3	D	501	PLP	C5-C4	2.53	1.43	1.40
3	D	501	PLP	C2A-C2	-2.51	1.46	1.50
3	A	502	PLP	C6-N1	2.33	1.39	1.34
4	B	501	GOL	O2-C2	-2.32	1.36	1.43
3	B	502	PLP	C6-N1	2.28	1.39	1.34
3	A	502	PLP	C2A-C2	-2.20	1.46	1.50
3	A	502	PLP	C3-C4	2.12	1.44	1.40
3	A	502	PLP	P-O1P	2.09	1.57	1.50
3	D	501	PLP	P-O1P	2.09	1.57	1.50
3	C	503	PLP	O3-C3	-2.04	1.32	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	PLP	C4A-C4-C5	5.75	126.87	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PLP	C6-C5-C4	5.43	122.55	118.10
3	D	501	PLP	O4P-C5A-C5	4.53	117.84	109.36
3	A	502	PLP	O3P-P-O2P	3.67	121.55	107.80
3	A	502	PLP	O4P-C5A-C5	3.24	115.43	109.36
3	A	502	PLP	C4A-C4-C5	3.16	124.20	120.94
3	C	503	PLP	C6-N1-C2	3.12	124.85	119.20
3	C	503	PLP	C6-C5-C4	3.10	120.64	118.10
3	B	502	PLP	O3P-P-O4P	-3.05	98.72	106.67
3	D	501	PLP	O3P-P-O2P	2.94	118.81	107.80
3	A	502	PLP	C3-C4-C5	-2.73	115.32	118.59
3	C	503	PLP	C2A-C2-N1	2.48	122.32	117.64
3	D	501	PLP	C2A-C2-N1	2.40	122.16	117.64
3	D	501	PLP	C4A-C4-C3	-2.37	116.57	120.52
3	B	502	PLP	C6-N1-C2	2.36	123.47	119.20
3	C	503	PLP	O3-C3-C2	2.30	122.34	117.58
4	B	501	GOL	O2-C2-C3	-2.28	99.75	109.18
3	B	502	PLP	O4P-P-O1P	-2.28	100.29	106.44
3	A	502	PLP	C5A-C5-C4	-2.26	118.18	122.64
3	C	503	PLP	O4P-P-O1P	-2.21	100.46	106.44
3	C	503	PLP	C4-C3-C2	-2.19	116.61	119.89
4	B	501	GOL	C3-C2-C1	2.15	119.69	111.80
3	A	502	PLP	O3P-P-O4P	-2.04	101.34	106.67
3	A	502	PLP	O3-C3-C4	2.04	123.43	118.10
3	C	503	PLP	C2A-C2-C3	-2.01	118.45	120.80

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	461/463 (99%)	-0.23	8 (1%) 69 74	6, 17, 33, 65	14 (3%)
1	B	462/463 (99%)	-0.02	6 (1%) 75 80	8, 19, 33, 86	12 (2%)
1	C	462/463 (99%)	-0.13	7 (1%) 72 77	5, 17, 31, 51	10 (2%)
1	D	463/463 (100%)	-0.26	8 (1%) 69 74	6, 15, 28, 84	16 (3%)
All	All	1848/1852 (99%)	-0.16	29 (1%) 70 75	5, 17, 31, 86	52 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PHE	9.7
1	D	11	PHE	8.0
1	D	10	GLY	7.1
1	C	11	PHE	5.5
1	B	472	LYS	4.7
1	B	435[A]	MET	4.4
1	A	11	PHE	4.3
1	D	12	ASP	4.0
1	D	472	LYS	3.8
1	B	12	ASP	3.8
1	D	435[A]	MET	3.6
1	C	472	LYS	3.1
1	C	17	LEU	3.1
1	A	157	GLY	2.8
1	A	163	LYS	2.7
1	C	435[A]	MET	2.7
1	B	180	TYR	2.6
1	B	228	GLU	2.4
1	C	256	LYS	2.4
1	C	12	ASP	2.4
1	D	14	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	180	TYR	2.3
1	A	12	ASP	2.3
1	D	441	ASP	2.3
1	D	240[A]	ARG	2.2
1	A	158	GLU	2.1
1	A	435[A]	MET	2.1
1	A	441	ASP	2.1
1	C	441	ASP	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
4	GOL	B	501	6/6	0.86	0.16	23,38,46,49	0
4	GOL	C	502	6/6	0.86	0.14	36,47,48,48	0
3	PLP	B	502	15/16	0.97	0.07	13,16,19,22	0
3	PLP	D	501	15/16	0.98	0.06	10,14,17,24	0
3	PLP	C	503	15/16	0.99	0.04	10,12,15,21	0
3	PLP	A	502	15/16	0.99	0.04	12,15,19,20	0
2	FES	A	501	4/4	1.00	0.02	13,13,13,13	0
2	FES	C	501	4/4	1.00	0.02	11,11,11,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.