Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:00 AM GMT

PDB ID	:	2VMY
Title	:	CRYSTAL STRUCTURE OF F351GBSSHMT IN COMPLEX WITH GLY AND FTHF
Authors	:	Rajaram, V.; Pai, V.R.; Bisht, S.; Bhavani, B.S.; Appaji Rao, N.; Savithri, H.S.; Murthy, M.R.N.
Deposited on	:	2008-01-29
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

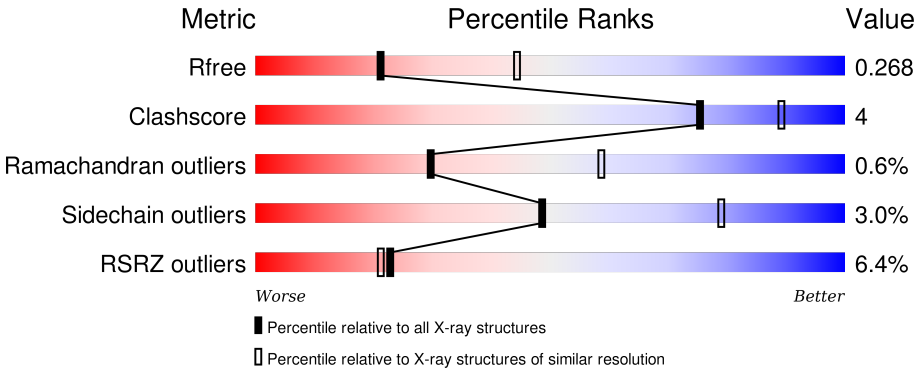
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	405	7% 88% 11%
1	B	405	6% 91% 9%

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
5	MRD	B	701	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6364 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.

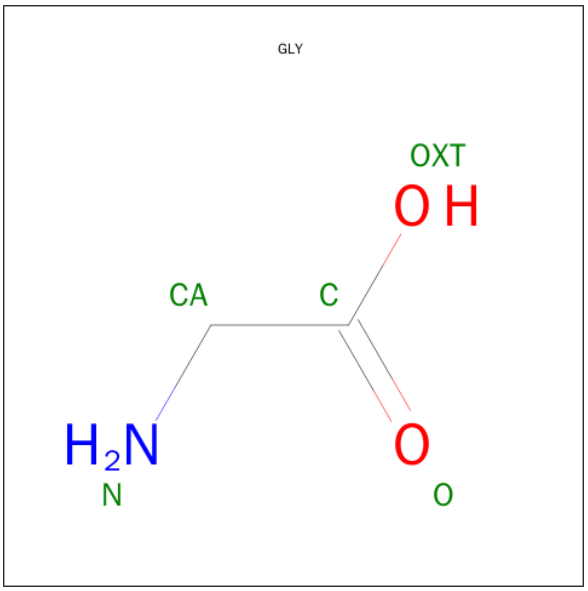
- Molecule 1 is a protein called SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	1	0
			3115	1967	551	586	11			
1	B	405	Total	C	N	O	S	0	0	0
			3109	1963	551	584	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	GLY	PHE	ENGINEERED MUTATION	UNP Q7SIB6
B	351	GLY	PHE	ENGINEERED MUTATION	UNP Q7SIB6

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



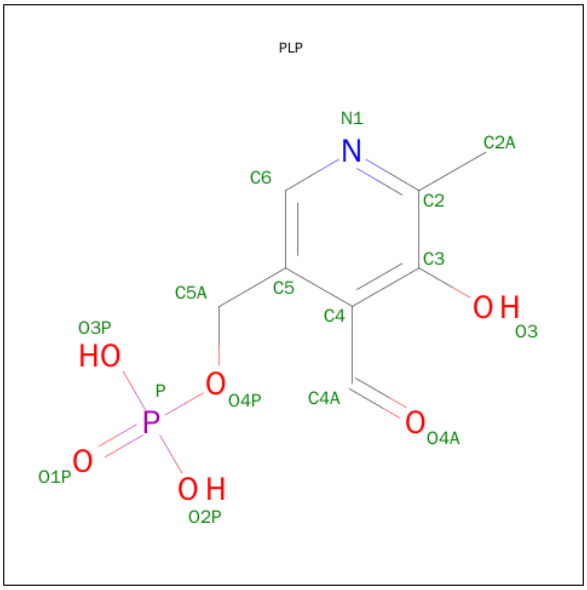
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

Continued on next page...

Continued from previous page...

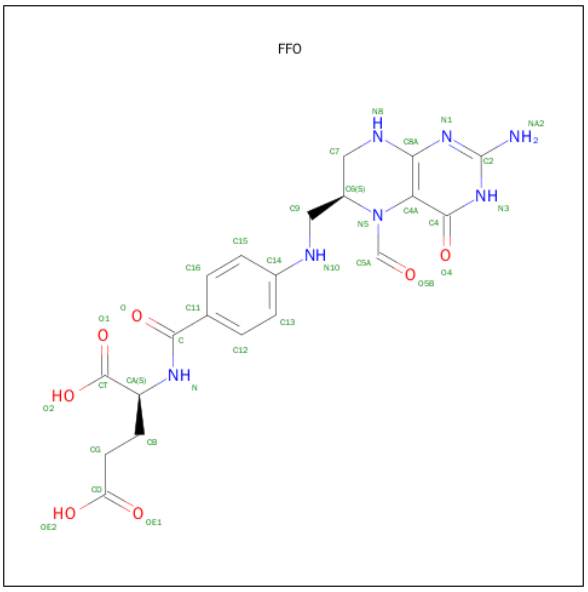
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

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



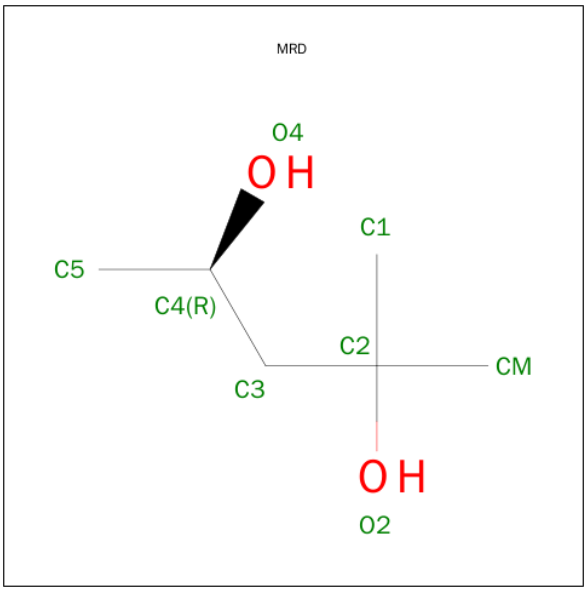
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is N-[4-({[(6S)-2-AMINO-5-FORMYL-4-OXO-3,4,5,6,7,8-HEXAHYDROPTERIDIN-6-YL]METHYL}AMINO)BENZOYL]-L-GLUTAMIC ACID (three-letter code: FFO) (formula: $C_{20}H_{23}N_7O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 34 20 7 7	0	0
4	B	1	Total C N O 34 20 7 7	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 8 6 2	0	0

- Molecule 6 is water.

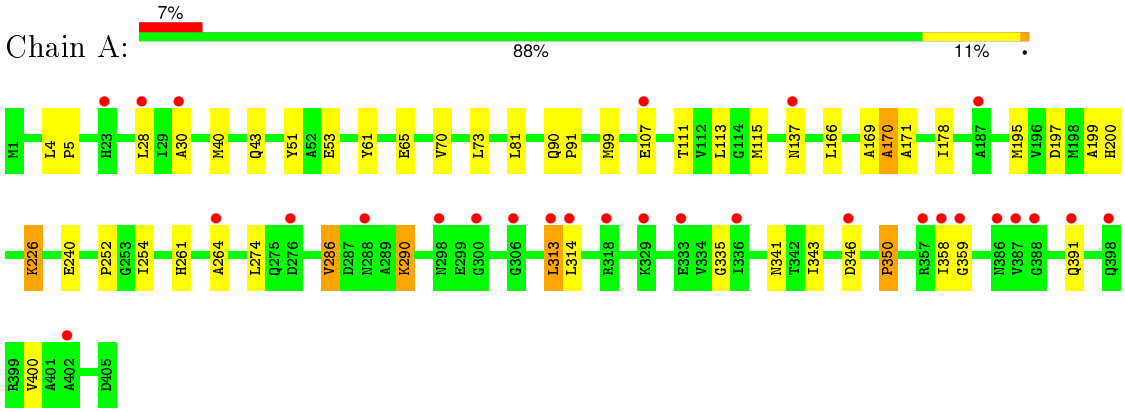
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

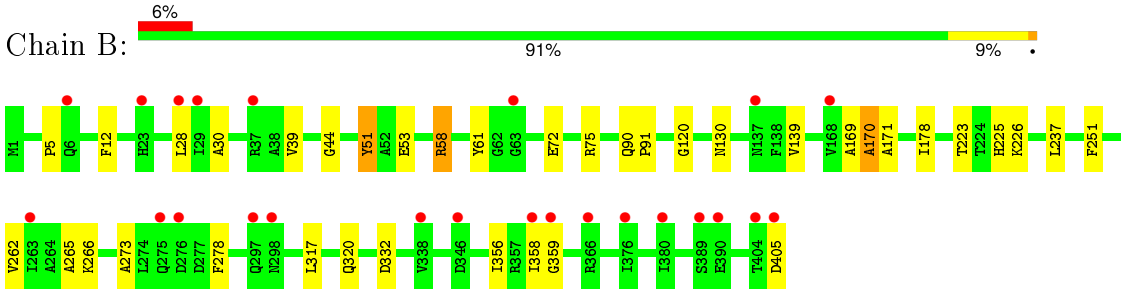
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain A:



- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.38Å 103.48Å 61.96Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	20.81 – 2.70 20.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.81-2.70) 98.7 (20.81-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.263 0.215 , 0.268	Depositor DCC
R_{free} test set	1007 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.1	EDS
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 19661 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, FFO, 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	0.33	0/3180	0.50	1/4310 (0.0%)
1	B	0.33	0/3171	0.49	0/4298
All	All	0.33	0/6351	0.50	1/8608 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3115	0	3095	25	0
1	B	3109	0	3089	21	0
2	A	5	0	2	3	0
2	B	5	0	2	2	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
4	A	34	0	21	2	0
4	B	34	0	21	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	8	0	14	0	0
6	A	12	0	0	0	0
6	B	12	0	0	0	0
All	All	6364	0	6258	49	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 (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:GLY:N	3:B:501:PLP:HO3	1.81	0.79
2:A:502:GLY:N	3:A:501:PLP:HO3	1.79	0.78
1:A:30:ALA:HA	1:A:359:GLY:HA3	1.81	0.63
1:A:166:LEU:HD11	1:A:195:MET:HB2	1.80	0.63
1:B:30:ALA:HA	1:B:359:GLY:HA3	1.80	0.63
1:A:169:ALA:O	1:A:170:ALA:CB	2.50	0.58
1:B:170:ALA:HA	1:B:178:ILE:HD13	1.85	0.57
1:B:28:LEU:HB3	1:B:358:ILE:HG23	1.86	0.57
1:B:53:GLU:HB2	1:B:61:TYR:HE2	1.71	0.56
1:A:90:GLN:N	1:A:91:PRO:CD	2.69	0.55
1:B:39:VAL:HG13	1:B:265:ALA:HB1	1.88	0.55
1:B:169:ALA:O	1:B:170:ALA:HB3	2.06	0.54
1:A:350:PRO:HG2	4:B:505:FFO:HB1	1.90	0.53
1:A:53:GLU:HB2	1:A:61:TYR:HE2	1.73	0.53
1:A:28:LEU:HB3	1:A:358:ILE:HG23	1.91	0.52
1:B:90:GLN:N	1:B:91:PRO:CD	2.71	0.52
1:A:81:LEU:HD13	1:A:274:LEU:HG	1.92	0.51
1:A:170:ALA:HA	1:A:178:ILE:HD13	1.92	0.51
1:A:169:ALA:O	1:A:170:ALA:HB3	2.10	0.50
1:A:99:MET:HE3	1:A:254:ILE:HB	1.93	0.50
1:A:335:GLY:HA3	1:A:400:VAL:HG11	1.94	0.50
1:A:43:GLN:HA	1:A:261:HIS:HB2	1.95	0.49
1:B:169:ALA:O	1:B:170:ALA:CB	2.60	0.49
1:A:40:MET:HB3	1:B:44:GLY:O	2.12	0.48
1:A:170:ALA:HB1	1:A:197:ASP:O	2.13	0.48
1:A:286:VAL:HG13	1:A:290:LYS:HZ2	1.78	0.48
1:A:252:PRO:O	1:B:130:ASN:ND2	2.37	0.48
1:A:4:LEU:N	1:A:5:PRO:HD2	2.29	0.48
1:A:200:HIS:HA	1:A:226:LYS:HD2	1.95	0.47
1:A:286:VAL:HG13	1:A:290:LYS:NZ	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:502:GLY:HA2	1:B:51:TYR:CZ	2.50	0.47
1:B:72:GLU:OE1	1:B:75:ARG:NH2	2.45	0.46
1:A:343:ILE:O	1:A:346:ASP:HB2	2.16	0.46
1:B:58:ARG:HD3	1:B:58:ARG:O	2.17	0.45
1:B:120:GLY:O	1:B:171:ALA:HB1	2.17	0.45
1:A:70:VAL:HG13	1:A:264:ALA:HA	2.00	0.44
1:B:317:LEU:HD11	1:B:356:ILE:HG12	2.00	0.44
4:A:505:FFO:O5B	2:B:502:GLY:HA3	2.18	0.43
1:A:115:MET:SD	1:A:171:ALA:HB2	2.59	0.43
4:A:505:FFO:H5A	4:A:505:FFO:O4	2.18	0.43
1:B:5:PRO:HG3	1:B:12:PHE:CE1	2.53	0.43
2:A:502:GLY:HA3	4:B:505:FFO:H5A	2.02	0.42
1:A:111:THR:HA	1:A:137:ASN:O	2.20	0.42
1:B:273:ALA:HA	1:B:278:PHE:CG	2.55	0.42
1:B:53:GLU:HB2	1:B:61:TYR:CE2	2.52	0.41
1:A:199:ALA:HB1	1:A:226:LYS:HE2	2.02	0.41
1:B:262:VAL:HG12	1:B:266:LYS:HE3	2.02	0.41
1:B:223:THR:HB	1:B:225:HIS:CE1	2.56	0.41
1:B:251:PHE:HZ	4:B:505:FFO:H15	1.86	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	404/405 (100%)	390 (96%)	11 (3%)	3 (1%)	26	55
1	B	403/405 (100%)	390 (97%)	11 (3%)	2 (0%)	34	63
All	All	807/810 (100%)	780 (97%)	22 (3%)	5 (1%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	B	170	ALA
1	A	226	LYS
1	B	226	LYS
1	A	350	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	321/320 (100%)	309 (96%)	12 (4%)	41 72
1	B	320/320 (100%)	313 (98%)	7 (2%)	60 86
All	All	641/640 (100%)	622 (97%)	19 (3%)	48 79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	65	GLU
1	A	73	LEU
1	A	107	GLU
1	A	113	LEU
1	A	240	GLU
1	A	286	VAL
1	A	290	LYS
1	A	313	LEU
1	A	314	LEU
1	A	341	ASN
1	A	391	GLN
1	B	51	TYR
1	B	58	ARG
1	B	139	VAL
1	B	237	LEU
1	B	320	GLN
1	B	332	ASP
1	B	405	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	239	GLN
1	A	275	GLN
1	A	391	GLN
1	A	398	GLN
1	B	17	GLN
1	B	43	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
3	PLP	A	501	2	15,15,16	1.06	2 (13%)	21,22,23	1.05	2 (9%)
2	GLY	A	502	3	1,4,4	0.54	0	0,4,4	0.00	-
4	FFO	A	505	-	27,36,36	1.99	6 (22%)	30,50,50	1.74	7 (23%)
3	PLP	B	501	2	15,15,16	0.93	1 (6%)	21,22,23	1.10	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLY	B	502	3	1,4,4	0.49	0	0,4,4	0.00	-
4	FFO	B	505	-	27,36,36	2.02	5 (18%)	30,50,50	1.74	6 (20%)
5	MRD	B	701	-	6,7,7	0.28	0	7,10,10	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	501	2	-	0/6/6/8	0/1/1/1
2	GLY	A	502	3	-	0/0/2/2	0/0/0/0
4	FFO	A	505	-	-	0/18/37/37	0/2/3/3
3	PLP	B	501	2	-	0/6/6/8	0/1/1/1
2	GLY	B	502	3	-	0/0/2/2	0/0/0/0
4	FFO	B	505	-	-	0/18/37/37	0/2/3/3
5	MRD	B	701	-	-	0/5/5/5	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	FFO	C7-N8	-3.42	1.41	1.46
4	A	505	FFO	C7-N8	-3.05	1.42	1.46
4	A	505	FFO	C11-C	2.03	1.54	1.50
3	A	501	PLP	C6-N1	2.04	1.38	1.34
3	B	501	PLP	C2-N1	2.24	1.38	1.34
3	A	501	PLP	C2-N1	2.38	1.39	1.34
4	A	505	FFO	C2-N3	2.78	1.40	1.35
4	B	505	FFO	C2-N3	2.92	1.40	1.35
4	A	505	FFO	C4-N3	3.79	1.40	1.33
4	B	505	FFO	C4-N3	4.02	1.40	1.33
4	A	505	FFO	O4-C4	5.25	1.37	1.24
4	B	505	FFO	O4-C4	5.31	1.37	1.24
4	B	505	FFO	C5A-N5	5.85	1.48	1.36
4	A	505	FFO	C5A-N5	5.86	1.48	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	505	FFO	N3-C2-N1	-3.43	119.91	125.53
4	B	505	FFO	O5B-C5A-N5	-3.41	119.09	124.21
4	A	505	FFO	N3-C2-N1	-3.38	119.99	125.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	505	FFO	C4A-C4-N3	-3.03	118.79	123.46
4	B	505	FFO	C4A-C4-N3	-2.84	119.08	123.46
3	B	501	PLP	C5-C6-N1	-2.26	119.94	123.86
4	A	505	FFO	O5B-C5A-N5	-2.19	120.92	124.21
3	A	501	PLP	C5-C6-N1	-2.14	120.15	123.86
4	A	505	FFO	NA2-C2-N1	2.04	120.58	117.20
3	B	501	PLP	C6-C5-C4	2.23	120.04	118.15
3	A	501	PLP	O4P-C5A-C5	2.58	113.27	108.99
4	B	505	FFO	C4-N3-C2	2.64	119.60	115.94
3	B	501	PLP	O4P-C5A-C5	2.70	113.46	108.99
4	A	505	FFO	C4-N3-C2	2.73	119.72	115.94
4	A	505	FFO	C2-N1-C8A	3.03	121.34	114.54
4	B	505	FFO	C2-N1-C8A	3.19	121.72	114.54
4	B	505	FFO	C4-C4A-C8A	5.26	118.62	114.43
4	A	505	FFO	C4-C4A-C8A	6.09	119.28	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PLP	1	0
2	A	502	GLY	3	0
4	A	505	FFO	2	0
3	B	501	PLP	1	0
2	B	502	GLY	2	0
4	B	505	FFO	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^{th} 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	405/405 (100%)	0.34	28 (6%)	20	18	45, 57, 73, 76	0
1	B	405/405 (100%)	0.24	24 (5%)	26	24	47, 56, 67, 71	0
All	All	810/810 (100%)	0.29	52 (6%)	23	21	45, 57, 70, 76	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	ILE	4.9
1	B	358	ILE	4.2
1	A	28	LEU	4.1
1	B	28	LEU	4.1
1	A	388	GLY	4.0
1	A	23	HIS	3.5
1	A	359	GLY	3.4
1	B	6	GLN	3.1
1	B	63	GLY	3.1
1	A	391	GLN	2.9
1	A	300	GLY	2.8
1	B	298	ASN	2.7
1	B	389	SER	2.7
1	A	276	ASP	2.6
1	A	402	ALA	2.6
1	A	329	LYS	2.6
1	B	275	GLN	2.6
1	A	357	ARG	2.6
1	A	137	ASN	2.5
1	B	366	ARG	2.5
1	A	107	GLU	2.5
1	B	137	ASN	2.5
1	B	276	ASP	2.4
1	A	387	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	404	THR	2.4
1	A	314	LEU	2.4
1	A	313	LEU	2.4
1	B	23	HIS	2.3
1	B	405	ASP	2.3
1	A	298	ASN	2.3
1	B	168	VAL	2.3
1	B	29	ILE	2.3
1	B	390	GLU	2.2
1	A	30	ALA	2.2
1	B	359	GLY	2.2
1	B	263	ILE	2.2
1	B	338	VAL	2.2
1	A	288	ASN	2.2
1	B	297	GLN	2.2
1	A	386	ASN	2.2
1	B	37	ARG	2.2
1	A	264	ALA	2.2
1	A	346	ASP	2.2
1	A	336	ILE	2.1
1	A	398	GLN	2.1
1	A	187	ALA	2.1
1	B	346	ASP	2.1
1	B	380	ILE	2.1
1	A	333	GLU	2.1
1	A	306	GLY	2.1
1	B	376	ILE	2.0
1	A	318	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MRD	B	701	8/8	0.91	0.30	3.12	57,57,57,57	0
3	PLP	A	501	15/16	0.93	0.23	1.25	48,50,50,50	0
3	PLP	B	501	15/16	0.95	0.19	0.98	49,52,52,52	0
2	GLY	A	502	5/5	0.92	0.24	0.34	50,50,50,50	0
2	GLY	B	502	5/5	0.95	0.17	-0.40	52,52,52,52	0
4	FFO	B	505	34/34	0.92	0.16	-0.43	59,60,61,62	0
4	FFO	A	505	34/34	0.94	0.14	-0.71	59,60,62,63	0

6.5 Other polymers (i)

There are no such residues in this entry.