



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 03:03 pm GMT

PDB ID : 1RV3  
Title : E75L MUTANT OF RABBIT CYTOSOLIC SERINE HYDROXYMETHYL  
TRANSFERASE, COMPLEX WITH GLYCINE  
Authors : Szebenyi, D.M.; Musayev, F.N.; di Salvo, M.L.; Safo, M.K.; Schirch, V.  
Deposited on : 2003-12-12  
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

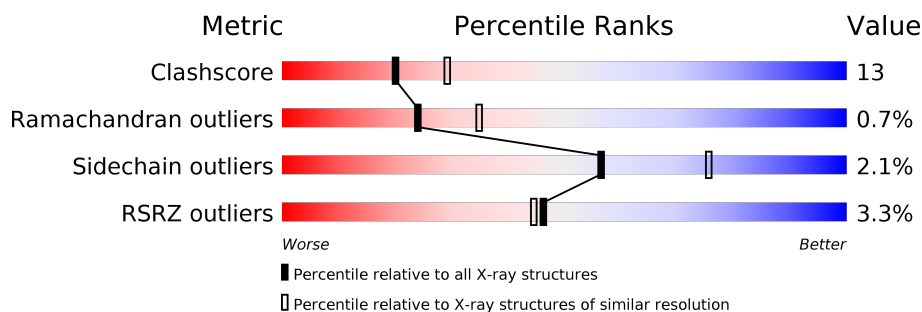
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	483	<div> <div>3%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
1	B	483	<div> <div>3%</div> <div>73%</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
3	PLP	A	500	-	X	-	-
4	GLY	B	602[C]	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7327 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.

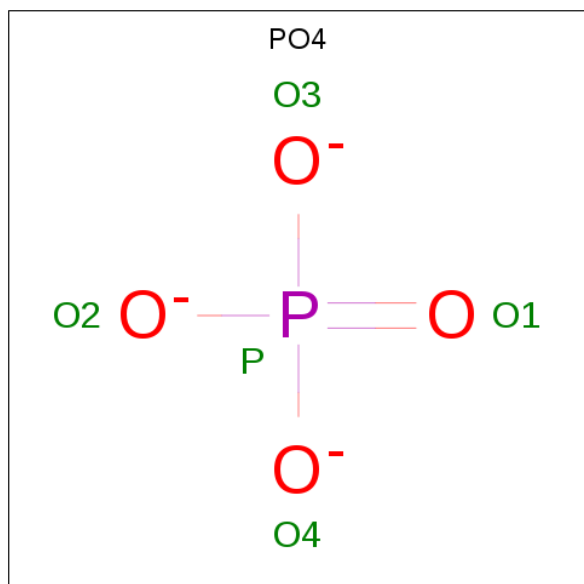
- Molecule 1 is a protein called Serine hydroxymethyltransferase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	1	0
			3587	2260	640	669	18			
1	B	466	Total	C	N	O	S	0	0	0
			3604	2269	644	673	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	LEU	GLU	ENGINEERED	UNP P07511
B	75	LEU	GLU	ENGINEERED	UNP P07511

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



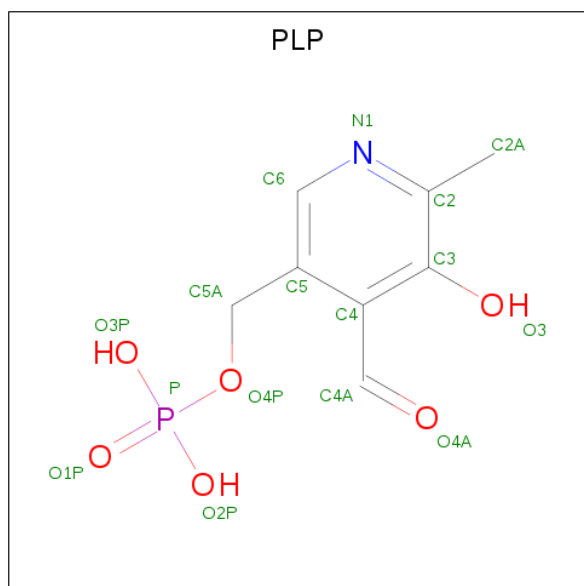
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

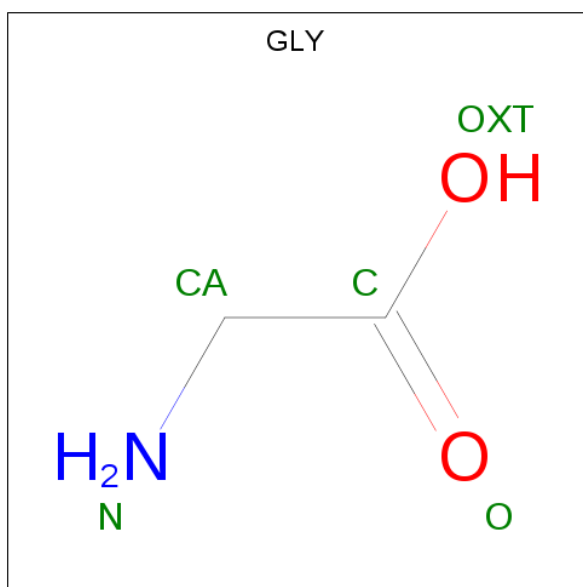
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	1
			5	4	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			10	4	2	4		

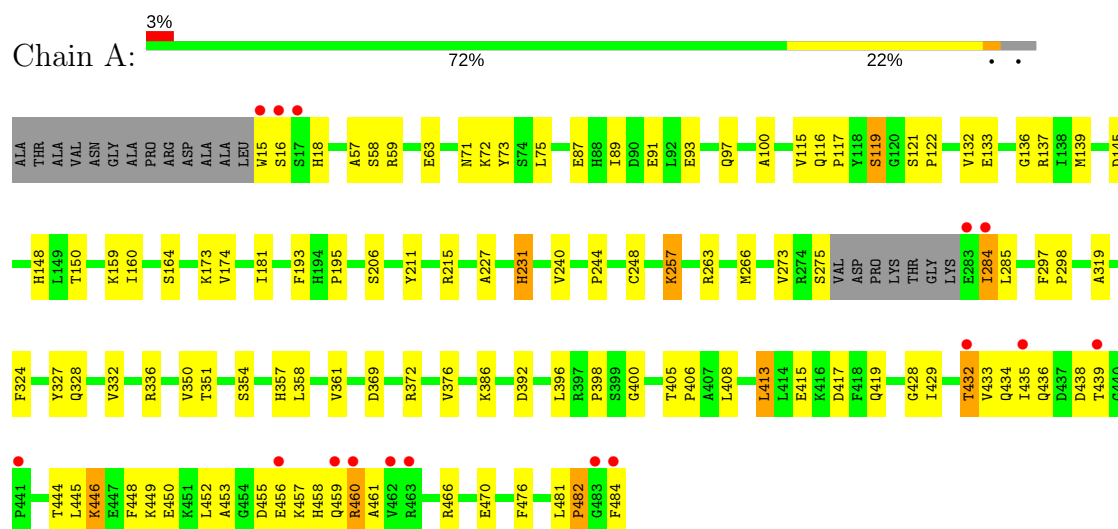
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	43	Total	O	0	0
			43	43		

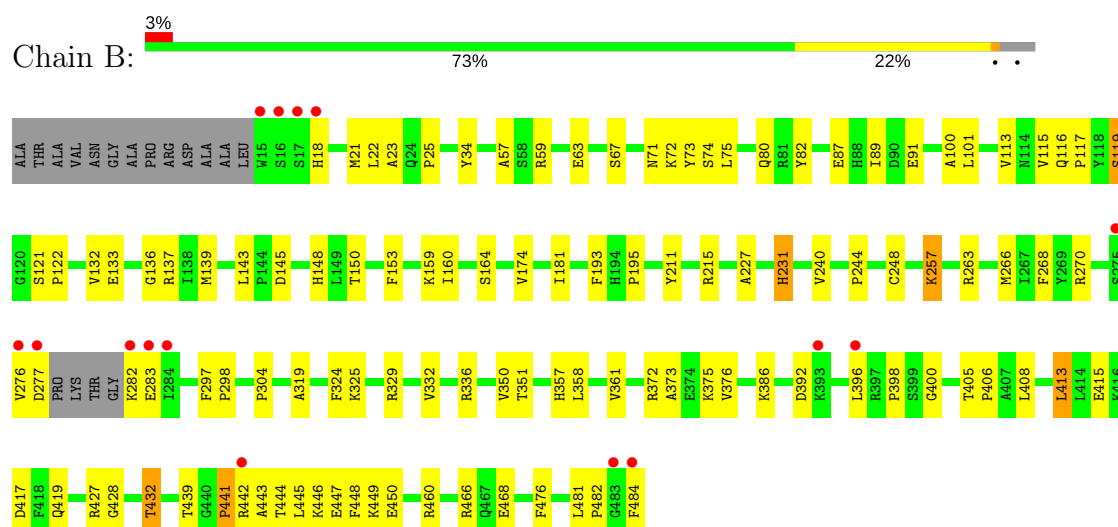
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Serine hydroxymethyltransferase, cytosolic



- Molecule 1: Serine hydroxymethyltransferase, cytosolic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.92Å 114.92Å 158.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.40 48.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.88-2.40) 98.7 (48.88-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.255 0.216 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: PO4, 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	0.36	0/3666	0.61	3/4954 (0.1%)
1	B	0.37	0/3677	0.61	3/4968 (0.1%)
All	All	0.36	0/7343	0.61	6/9922 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	LYS	CD-CE-NZ	7.40	128.72	111.70
1	A	460	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	460	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	257	LYS	CD-CE-NZ	6.05	125.62	111.70
1	A	460	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	460	ARG	NE-CZ-NH2	5.86	123.23	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3587	0	3565	102	0
1	B	3604	0	3586	103	0
2	A	5	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	15	0	6	1	0
3	B	15	0	6	1	0
4	B	10	0	4	6	0
5	A	43	0	0	0	0
5	B	43	0	0	0	0
All	All	7327	0	7167	194	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 13.

All (194) 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:101:LEU:HD21	1:B:113:VAL:HG23	1.55	0.87
1:A:15:TRP:HD1	1:A:16:SER:H	1.24	0.83
1:B:257:LYS:HE3	4:B:602[C]:GLY:HA3	1.61	0.82
1:B:74:SER:O	1:B:304:PRO:HD2	1.80	0.81
1:B:325:LYS:HE3	1:B:329:ARG:HH22	1.45	0.81
1:A:386:LYS:HD2	1:A:398:PRO:HG3	1.63	0.80
1:A:115:VAL:HG12	1:A:266:MET:HE3	1.63	0.79
1:A:72:LYS:HG2	1:A:89:ILE:HG13	1.67	0.76
1:B:115:VAL:HG12	1:B:266:MET:HE3	1.68	0.75
1:B:386:LYS:HD2	1:B:398:PRO:HG3	1.67	0.74
1:B:441:PRO:HG2	1:B:442:ARG:H	1.52	0.73
1:B:444:THR:HG23	1:B:447:GLU:H	1.54	0.73
1:A:73[A]:TYR:HD1	1:B:263:ARG:HH22	1.35	0.72
1:A:428:GLY:O	1:A:432:THR:HG23	1.90	0.71
1:A:456:GLU:HB3	1:A:460:ARG:HH22	1.56	0.70
1:A:100:ALA:HB2	1:A:266:MET:HE1	1.73	0.70
1:A:433:VAL:O	1:A:436:GLN:HB3	1.91	0.70
1:B:100:ALA:HB2	1:B:266:MET:HE1	1.73	0.69
1:A:456:GLU:HB3	1:A:460:ARG:NH2	2.08	0.68
1:A:484:PHE:CZ	1:B:67:SER:HA	2.28	0.68
1:B:59:ARG:HG3	1:B:481:LEU:HD23	1.76	0.67
1:A:453:ALA:HA	1:A:459:GLN:NE2	2.10	0.67
1:B:428:GLY:O	1:B:432:THR:HG23	1.96	0.66
1:B:282:LYS:HE2	1:B:282:LYS:HA	1.77	0.65
1:B:446:LYS:O	1:B:450:GLU:HG3	1.96	0.65
1:A:115:VAL:HG12	1:A:266:MET:CE	2.28	0.64
1:B:376:VAL:CB	1:B:432:THR:HG22	2.27	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:CE	4:B:602[C]:GLY:HA3	2.28	0.63
1:B:445:LEU:HG	1:B:449:LYS:HE3	1.80	0.63
1:A:72:LYS:HG2	1:A:89:ILE:CG1	2.29	0.62
1:B:376:VAL:HB	1:B:432:THR:HG22	1.81	0.62
1:B:325:LYS:HE3	1:B:329:ARG:NH2	2.12	0.62
1:A:376:VAL:HB	1:A:432:THR:HG22	1.82	0.62
1:A:59:ARG:CZ	1:B:25:PRO:HG3	2.30	0.61
1:B:240:VAL:HG11	1:B:332:VAL:HG21	1.83	0.61
1:B:159:LYS:HD3	1:B:164:SER:O	2.01	0.61
1:B:413:LEU:HD22	1:B:476:PHE:CE2	2.37	0.60
1:B:444:THR:HG22	1:B:447:GLU:HG3	1.82	0.60
1:A:376:VAL:CB	1:A:432:THR:HG22	2.31	0.59
1:B:115:VAL:HG12	1:B:266:MET:CE	2.33	0.59
1:B:132:VAL:O	1:B:133:GLU:HB2	2.03	0.59
1:B:59:ARG:O	1:B:63:GLU:HG3	2.02	0.59
1:A:435:ILE:HD13	1:A:452:LEU:HD13	1.84	0.59
1:A:240:VAL:HG11	1:A:332:VAL:HG21	1.84	0.58
1:A:275:SER:HB3	1:A:284:ILE:HD11	1.84	0.58
1:A:59:ARG:O	1:A:63:GLU:HG3	2.04	0.58
1:A:121:SER:HB2	1:A:122:PRO:HD3	1.87	0.57
1:B:257:LYS:HE3	4:B:602[B]:GLY:HA2	1.87	0.57
1:A:458:HIS:O	1:A:461:ALA:N	2.37	0.57
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.70	0.57
1:B:405:THR:N	1:B:406:PRO:CD	2.68	0.57
1:B:444:THR:CG2	1:B:447:GLU:HG3	2.35	0.56
1:A:231:HIS:HD2	1:A:357:HIS:NE2	2.02	0.56
1:B:145:ASP:HB3	1:B:174:VAL:HG13	1.87	0.56
1:A:139:MET:HG3	1:A:195:PRO:HB3	1.87	0.56
1:A:446:LYS:O	1:A:450:GLU:HG3	2.05	0.56
1:A:405:THR:N	1:A:406:PRO:CD	2.69	0.56
1:B:121:SER:HB2	1:B:122:PRO:HD3	1.88	0.56
1:A:275:SER:HB3	1:A:284:ILE:CD1	2.36	0.56
1:B:113:VAL:HG22	1:B:268:PHE:CD1	2.41	0.56
1:B:148:HIS:HD2	1:B:150:THR:OG1	1.88	0.56
1:A:413:LEU:HD22	1:A:476:PHE:CE2	2.41	0.55
1:B:72:LYS:HG2	1:B:89:ILE:HG13	1.88	0.55
1:A:57:ALA:H	1:B:71:ASN:HD21	1.54	0.55
1:B:257:LYS:HE2	3:B:600:PLP:O3	2.07	0.55
1:A:87:GLU:O	1:A:91:GLU:HG3	2.07	0.55
1:A:327:TYR:HB2	1:B:18:HIS:CD2	2.41	0.55
1:A:481:LEU:HD12	1:A:484:PHE:CE1	2.41	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:THR:N	1:B:406:PRO:HD3	2.22	0.55
1:A:435:ILE:CD1	1:A:452:LEU:HD13	2.36	0.55
1:B:231:HIS:HD2	1:B:357:HIS:NE2	2.05	0.54
1:B:336:ARG:HH11	1:B:336:ARG:HG3	1.73	0.54
1:B:375:LYS:HE3	1:B:449:LYS:HE2	1.89	0.54
1:A:275:SER:HB3	1:A:284:ILE:HG13	1.89	0.54
1:B:372:ARG:NH1	1:B:448:PHE:HB2	2.22	0.54
1:B:357:HIS:HD1	1:B:357:HIS:H	1.56	0.54
1:A:148:HIS:HD2	1:A:150:THR:OG1	1.90	0.53
1:A:137:ARG:HB3	1:A:193:PHE:CE2	2.44	0.53
1:A:415:GLU:O	1:A:419:GLN:HG3	2.09	0.53
1:A:160:ILE:HD12	1:A:160:ILE:N	2.23	0.53
1:B:277:ASP:HB3	1:B:282:LYS:HB3	1.91	0.53
1:A:145:ASP:HB3	1:A:174:VAL:HG13	1.90	0.52
1:A:159:LYS:HD3	1:A:164:SER:O	2.08	0.52
1:A:436:GLN:HA	1:A:439:THR:HG22	1.91	0.52
1:A:350:VAL:HG12	1:A:351:THR:HG23	1.90	0.52
1:A:139:MET:HE1	1:A:195:PRO:HG3	1.90	0.52
1:B:444:THR:HG22	1:B:447:GLU:CG	2.39	0.52
1:A:240:VAL:CG1	1:A:332:VAL:HG21	2.40	0.52
1:A:405:THR:N	1:A:406:PRO:HD3	2.25	0.52
1:B:160:ILE:HD12	1:B:160:ILE:N	2.24	0.52
1:A:408:LEU:HB3	1:A:413:LEU:HG	1.92	0.52
1:A:71:ASN:HD21	1:B:57:ALA:H	1.58	0.52
1:A:59:ARG:HD3	1:B:23:ALA:O	2.10	0.51
1:B:405:THR:H	1:B:406:PRO:HD3	1.75	0.51
1:B:415:GLU:O	1:B:419:GLN:HG3	2.09	0.51
1:A:132:VAL:O	1:A:133:GLU:HB2	2.10	0.51
1:A:275:SER:HB3	1:A:284:ILE:CG1	2.40	0.51
1:B:101:LEU:HD21	1:B:113:VAL:CG2	2.34	0.50
1:A:357:HIS:H	1:A:357:HIS:HD1	1.59	0.50
1:B:227:ALA:HB2	1:B:248:CYS:SG	2.52	0.50
1:B:240:VAL:CG1	1:B:332:VAL:HG21	2.40	0.50
1:B:211:TYR:CZ	1:B:244:PRO:HB3	2.47	0.50
1:B:257:LYS:CE	4:B:602[C]:GLY:CA	2.89	0.50
1:B:139:MET:HG3	1:B:195:PRO:HB3	1.93	0.49
1:B:257:LYS:HE3	4:B:602[C]:GLY:CA	2.39	0.49
1:A:455:ASP:OD1	1:A:457:LYS:HG2	2.13	0.49
1:A:458:HIS:C	1:A:460:ARG:N	2.62	0.49
1:B:231:HIS:HE1	4:B:602[B]:GLY:OXT	1.94	0.49
1:A:405:THR:H	1:A:406:PRO:HD3	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:O	1:B:91:GLU:HG3	2.14	0.48
1:A:115:VAL:CG1	1:A:266:MET:HE3	2.40	0.48
1:A:319:ALA:HA	1:A:324:PHE:CG	2.48	0.48
1:A:481:LEU:HD12	1:A:484:PHE:CZ	2.48	0.48
1:A:263:ARG:HH22	1:B:73:TYR:HD2	1.61	0.48
1:A:396:LEU:HD22	1:A:396:LEU:N	2.29	0.48
1:B:413:LEU:HD22	1:B:476:PHE:CZ	2.48	0.48
1:B:358:LEU:HD12	1:B:358:LEU:C	2.33	0.48
1:B:376:VAL:HG11	1:B:432:THR:HG22	1.96	0.48
1:A:15:TRP:CD1	1:A:16:SER:N	2.79	0.47
1:B:396:LEU:HD22	1:B:396:LEU:N	2.28	0.47
1:B:34:TYR:CE1	1:B:484:PHE:HE2	2.32	0.47
1:B:143:LEU:HD22	1:B:153:PHE:CD1	2.49	0.47
1:B:119:SER:C	1:B:122:PRO:HD2	2.35	0.47
1:B:439:THR:HG22	1:B:443:ALA:CB	2.45	0.47
1:A:413:LEU:HD13	1:A:417:ASP:HB3	1.96	0.47
1:B:148:HIS:CD2	1:B:150:THR:H	2.34	0.46
1:A:139:MET:CE	1:A:195:PRO:HG3	2.45	0.46
1:B:319:ALA:HA	1:B:324:PHE:CG	2.50	0.46
1:A:434:GLN:C	1:A:436:GLN:N	2.66	0.46
1:A:455:ASP:HB3	1:A:458:HIS:HB2	1.97	0.46
1:A:116:GLN:N	1:A:117:PRO:CD	2.78	0.46
1:A:206:SER:HB2	1:A:354:SER:HB2	1.98	0.46
1:A:148:HIS:CD2	1:A:150:THR:H	2.34	0.46
1:B:137:ARG:HB3	1:B:193:PHE:CE2	2.51	0.46
1:B:72:LYS:HG2	1:B:89:ILE:CG1	2.45	0.46
1:B:139:MET:HE2	1:B:195:PRO:HG3	1.98	0.46
1:A:211:TYR:CZ	1:A:244:PRO:HB3	2.50	0.46
1:B:372:ARG:HB3	1:B:448:PHE:CZ	2.50	0.45
1:B:441:PRO:HG2	1:B:442:ARG:N	2.26	0.45
1:B:376:VAL:CG1	1:B:432:THR:HG22	2.46	0.45
1:A:174:VAL:HA	1:A:181:ILE:HA	1.98	0.45
1:A:386:LYS:HD2	1:A:398:PRO:CG	2.42	0.45
1:B:116:GLN:N	1:B:117:PRO:CD	2.79	0.45
1:A:459:GLN:HA	1:A:459:GLN:NE2	2.32	0.45
1:B:270:ARG:HG2	1:B:270:ARG:HH11	1.81	0.45
1:B:297:PHE:CD1	1:B:298:PRO:HA	2.52	0.44
1:A:227:ALA:HB2	1:A:248:CYS:SG	2.58	0.44
1:A:435:ILE:HB	1:A:448:PHE:CE1	2.52	0.44
1:B:441:PRO:CG	1:B:442:ARG:H	2.24	0.44
1:B:350:VAL:HG12	1:B:351:THR:HG23	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:THR:OG1	1:A:446:LYS:HG3	2.17	0.44
1:A:273:VAL:HG22	1:A:285:LEU:CD2	2.48	0.44
1:B:18:HIS:O	1:B:21:MET:HB3	2.16	0.44
1:B:101:LEU:CD2	1:B:113:VAL:HG23	2.37	0.44
1:B:408:LEU:HB3	1:B:413:LEU:HG	1.99	0.43
1:A:57:ALA:H	1:B:71:ASN:ND2	2.15	0.43
1:A:458:HIS:C	1:A:460:ARG:H	2.22	0.43
1:B:361:VAL:O	1:B:400:GLY:HA2	2.18	0.43
1:A:434:GLN:C	1:A:436:GLN:H	2.21	0.43
1:A:361:VAL:O	1:A:400:GLY:HA2	2.19	0.43
1:B:113:VAL:CG2	1:B:268:PHE:CD1	3.01	0.43
1:A:358:LEU:HD12	1:A:358:LEU:C	2.38	0.43
1:A:372:ARG:HH12	1:A:445:LEU:HA	1.83	0.43
1:B:174:VAL:HA	1:B:181:ILE:HA	2.01	0.43
1:A:119:SER:C	1:A:122:PRO:HD2	2.39	0.42
1:A:100:ALA:CB	1:A:266:MET:HE1	2.45	0.42
1:B:413:LEU:HD13	1:B:417:ASP:HB3	2.01	0.42
1:B:139:MET:CE	1:B:195:PRO:HG3	2.49	0.42
1:A:145:ASP:OD2	1:A:173:LYS:HB3	2.20	0.42
1:A:72:LYS:CG	1:A:89:ILE:HG13	2.43	0.42
1:A:457:LYS:N	1:A:457:LYS:HD3	2.34	0.42
1:A:458:HIS:O	1:A:460:ARG:N	2.52	0.42
1:A:73[B]:TYR:HE2	1:A:75:LEU:HD21	1.83	0.42
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.90	0.42
1:B:132:VAL:HG12	1:B:136:GLY:HA3	2.01	0.42
1:A:132:VAL:HG12	1:A:136:GLY:HA3	2.02	0.42
1:A:297:PHE:CD1	1:A:298:PRO:HA	2.55	0.41
1:A:15:TRP:HB3	1:A:18:HIS:HB3	2.02	0.41
1:A:59:ARG:NH2	1:B:25:PRO:HG3	2.34	0.41
1:A:257:LYS:HE3	3:A:500:PLP:O3	2.20	0.41
1:A:466:ARG:O	1:A:470:GLU:HG3	2.21	0.41
1:B:75:LEU:HB2	1:B:82:TYR:HB2	2.01	0.41
1:B:80:GLN:HG2	1:B:80:GLN:O	2.21	0.41
1:B:441:PRO:CG	1:B:442:ARG:N	2.84	0.41
1:A:369:ASP:HB2	1:A:398:PRO:O	2.21	0.40
1:A:58:SER:HB3	1:B:22:LEU:HD23	2.04	0.40
1:B:427:ARG:HH22	1:B:468:GLU:CD	2.25	0.40
1:B:373:ALA:HA	1:B:432:THR:HG21	2.02	0.40
1:A:429:ILE:O	1:A:433:VAL:HG23	2.21	0.40
1:A:446:LYS:HA	1:A:449:LYS:HG2	2.03	0.40
1:A:481:LEU:O	1:A:482:PRO:C	2.60	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:PHE:CD1	1:B:484:PHE:OXT	2.75	0.40
1:A:93:GLU:O	1:A:97:GLN:HG3	2.21	0.40
1:B:59:ARG:HG3	1:B:481:LEU:CD2	2.46	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	460/483 (95%)	441 (96%)	17 (4%)	2 (0%)	36	51
1	B	462/483 (96%)	445 (96%)	13 (3%)	4 (1%)	19	27
All	All	922/966 (95%)	886 (96%)	30 (3%)	6 (1%)	24	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	ASP
1	B	392	ASP
1	B	441	PRO
1	A	482	PRO
1	B	276	VAL
1	B	482	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	379/391 (97%)	370 (98%)	9 (2%)	52	72
1	B	381/391 (97%)	374 (98%)	7 (2%)	62	79
All	All	760/782 (97%)	744 (98%)	16 (2%)	56	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	215	ARG
1	A	231	HIS
1	A	284	ILE
1	A	328	GLN
1	A	413	LEU
1	A	432	THR
1	A	438	ASP
1	A	446	LYS
1	B	119	SER
1	B	215	ARG
1	B	231	HIS
1	B	283	GLU
1	B	413	LEU
1	B	432	THR
1	B	466	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	102	GLN
1	A	109	GLN
1	A	148	HIS
1	A	231	HIS
1	A	287	ASN
1	A	328	GLN
1	A	459	GLN
1	A	467	GLN
1	B	71	ASN
1	B	102	GLN
1	B	109	GLN
1	B	148	HIS
1	B	231	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	287	ASN
1	B	328	GLN
1	B	459	GLN
1	B	467	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 ⓘ

6 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	500	1	15,15,16	5.49	10 (66%)	20,22,23	2.74	8 (40%)
2	PO4	A	501	-	4,4,4	1.34	0	6,6,6	0.38	0
3	PLP	B	600	1,4	15,15,16	5.57	10 (66%)	20,22,23	2.69	7 (35%)
2	PO4	B	601[A]	-	4,4,4	1.36	0	6,6,6	0.39	0
4	GLY	B	602[B]	3	1,4,4	0.16	0	0,4,4	0.00	-
4	GLY	B	602[C]	3	1,4,4	0.13	0	0,4,4	0.00	-

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	500	1	-	0/6/6/8	0/1/1/1
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
3	PLP	B	600	1,4	-	0/6/6/8	0/1/1/1
2	PO4	B	601[A]	-	-	0/0/0/0	0/0/0/0
4	GLY	B	602[B]	3	-	0/0/2/2	0/0/0/0
4	GLY	B	602[C]	3	-	0/0/2/2	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	PLP	P-O4P	-6.34	1.39	1.60
3	A	500	PLP	P-O4P	-6.27	1.40	1.60
3	B	600	PLP	C4A-C4	-6.13	1.39	1.51
3	A	500	PLP	C4A-C4	-5.31	1.40	1.51
3	B	600	PLP	P-O3P	-3.48	1.40	1.54
3	A	500	PLP	P-O3P	-3.37	1.41	1.54
3	B	600	PLP	P-O2P	-2.72	1.43	1.54
3	A	500	PLP	P-O2P	-2.53	1.44	1.54
3	B	600	PLP	C6-N1	2.31	1.39	1.34
3	A	500	PLP	C6-N1	2.53	1.39	1.34
3	A	500	PLP	C2-N1	3.89	1.41	1.33
3	B	600	PLP	C2-N1	3.99	1.41	1.33
3	B	600	PLP	C6-C5	4.10	1.46	1.37
3	A	500	PLP	C6-C5	4.38	1.46	1.37
3	A	500	PLP	C5-C4	6.82	1.48	1.40
3	A	500	PLP	C3-C4	6.98	1.55	1.40
3	B	600	PLP	C3-C4	7.26	1.55	1.40
3	B	600	PLP	C5-C4	7.62	1.49	1.40
3	B	600	PLP	C3-C2	14.76	1.51	1.40
3	A	500	PLP	C3-C2	15.15	1.51	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	PLP	C4A-C4-C5	-2.69	118.13	120.85
3	A	500	PLP	C4A-C4-C5	-2.55	118.27	120.85
3	A	500	PLP	C5-C6-N1	-2.43	119.71	123.83
3	B	600	PLP	C5-C6-N1	-2.41	119.75	123.83
3	A	500	PLP	C3-C2-N1	-2.08	118.01	120.75
3	B	600	PLP	C6-C5-C4	2.22	119.98	118.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLP	C6-C5-C4	2.36	120.10	118.19
3	B	600	PLP	O3-C3-C2	3.46	125.03	117.78
3	A	500	PLP	C6-N1-C2	3.55	126.04	119.19
3	B	600	PLP	C6-N1-C2	3.66	126.24	119.19
3	A	500	PLP	O3-C3-C2	3.72	125.57	117.78
3	B	600	PLP	O4P-C5A-C5	4.53	118.11	109.39
3	A	500	PLP	O4P-C5A-C5	5.06	119.12	109.39
3	A	500	PLP	O3P-P-O4P	7.83	127.57	106.73
3	B	600	PLP	O3P-P-O4P	7.84	127.61	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PLP	1	0
3	B	600	PLP	1	0
4	B	602[B]	GLY	2	0
4	B	602[C]	GLY	4	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	463/483 (95%)	-0.10	16 (3%) 44 42	23, 42, 96, 145	0
1	B	466/483 (96%)	-0.15	15 (3%) 47 46	20, 39, 94, 149	0
All	All	929/966 (96%)	-0.12	31 (3%) 46 44	20, 41, 97, 149	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	PHE	8.9
1	B	15	TRP	7.1
1	A	484	PHE	5.3
1	A	441	PRO	5.1
1	B	276	VAL	4.6
1	A	459	GLN	4.6
1	B	284	ILE	4.3
1	B	16	SER	4.2
1	B	483	GLY	4.1
1	B	18	HIS	4.1
1	B	277	ASP	4.0
1	A	435	ILE	3.5
1	B	17	SER	3.5
1	A	15	TRP	3.4
1	B	282	LYS	3.4
1	A	284	ILE	3.3
1	B	275	SER	3.0
1	B	396	LEU	3.0
1	B	442	ARG	2.9
1	A	463	ARG	2.6
1	A	283	GLU	2.5
1	B	283	GLU	2.5
1	A	483	GLY	2.4
1	A	462	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	16	SER	2.2
1	A	432	THR	2.2
1	A	17	SER	2.2
1	A	439	THR	2.2
1	B	393	LYS	2.2
1	A	456	GLU	2.1
1	A	460	ARG	2.1

## 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. 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(Å <sup>2</sup> )	Q<0.9
2	PO4	B	601[A]	5/5	0.90	0.23	38,39,40,41	5
4	GLY	B	602[B]	5/5	0.93	0.19	34,34,34,34	5
4	GLY	B	602[C]	5/5	0.93	0.19	44,44,44,44	5
3	PLP	A	500	15/16	0.94	0.19	43,46,49,49	0
3	PLP	B	600	15/16	0.94	0.18	50,53,55,57	0
2	PO4	A	501	5/5	0.96	0.15	76,76,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.