



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 12:29 AM EDT

PDB ID : 1RVU  
Title : E75Q MUTANT OF RABBIT CYTOSOLIC SERINE HYDROXYMETHYL  
TRANSFERASE  
Authors : Szebenyi, D.M.; Musayev, F.N.; Di Salvo, M.L.; Safo, M.K.; Schirch, V.  
Deposited on : 2003-12-15  
Resolution : 2.50 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

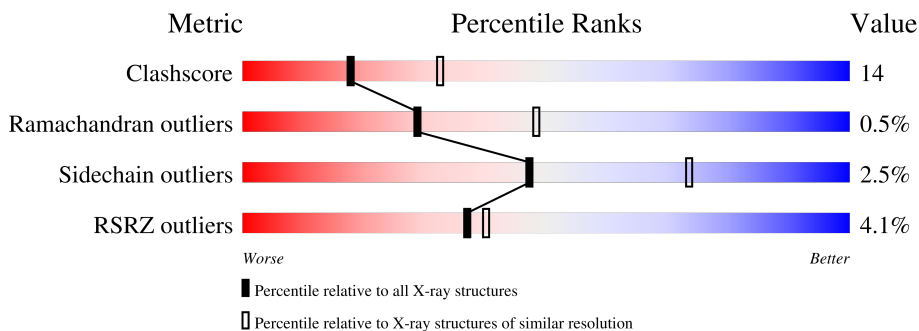
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	483	 5% 68% 26% . .
1	B	483	 3% 70% 25% . .

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
2	PLP	A	500	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7326 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.

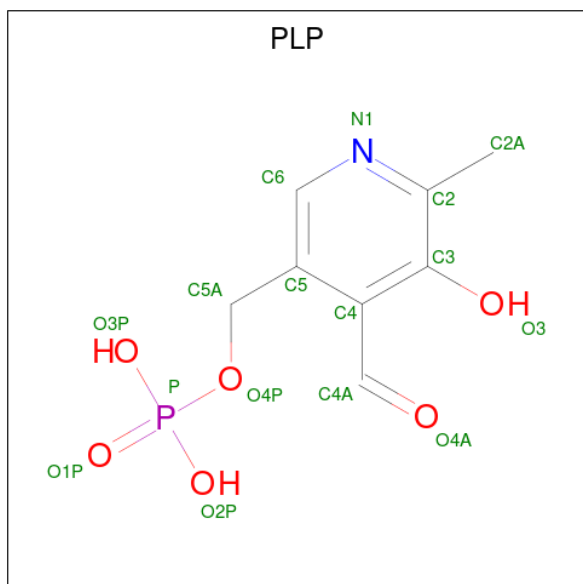
- Molecule 1 is a protein called Serine hydroxymethyltransferase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	Total 3581	C 2253	N 641	O 669	S 18	0	0	0
1	B	466	Total 3605	C 2268	N 645	O 674	S 18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLN	GLU	engineered mutation	UNP P07511
B	75	GLN	GLU	engineered mutation	UNP P07511

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

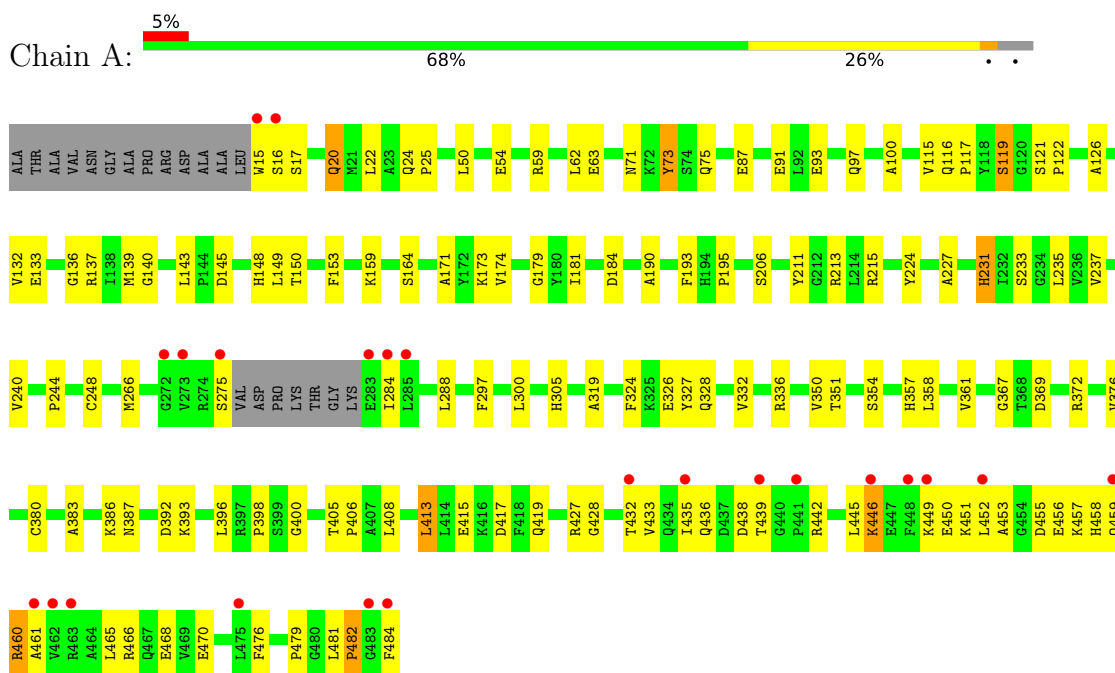
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	54	54	54	0	0
4	B	51	51	51	0	0

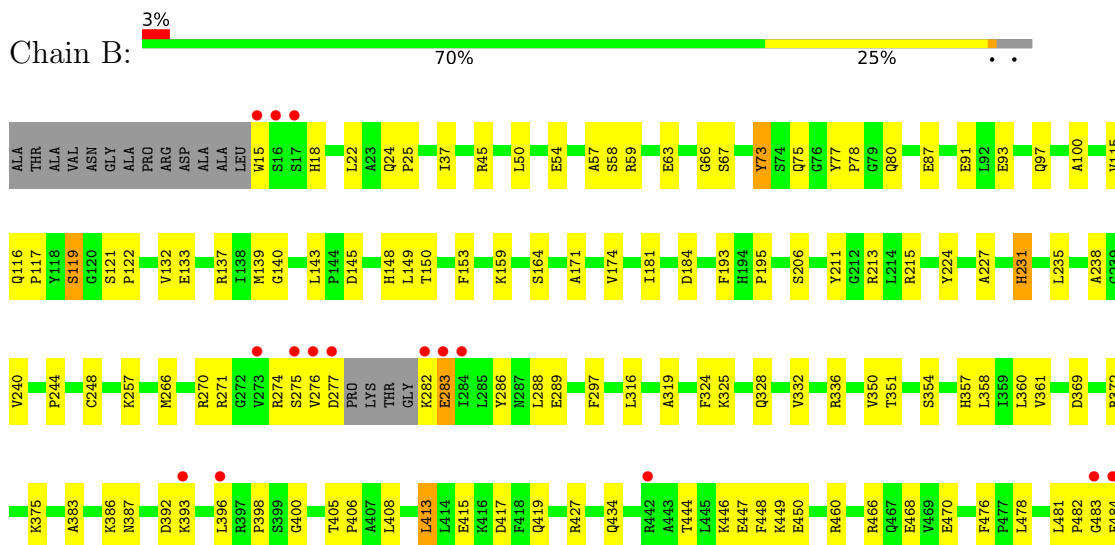
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	114.65Å 114.65Å 156.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.33 – 2.50 57.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (57.33-2.50) 99.5 (57.33-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.250 0.216 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: PLP, PO4

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	0.35	0/3654	0.61	2/4937 (0.0%)
1	B	0.35	0/3678	0.61	2/4969 (0.0%)
All	All	0.35	0/7332	0.61	4/9906 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	460	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	460	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	460	ARG	NE-CZ-NH2	5.67	123.13	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	3581	0	3557	109	0
1	B	3605	0	3583	98	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	54	0	0	0	0
4	B	51	0	0	0	0
All	All	7326	0	7152	196	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 14.

All (196) 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:275:SER:HB3	1:A:284:ILE:HD11	1.35	1.09
1:A:386:LYS:HD2	1:A:398:PRO:HG3	1.53	0.90
1:A:15:TRP:HD1	1:A:16:SER:H	1.18	0.88
1:B:413:LEU:HD13	1:B:417:ASP:HB3	1.63	0.81
1:B:386:LYS:HD2	1:B:398:PRO:HG3	1.61	0.80
1:A:413:LEU:HD13	1:A:417:ASP:HB3	1.64	0.79
1:A:428:GLY:O	1:A:432:THR:HG23	1.84	0.78
1:B:277:ASP:HB3	1:B:282:LYS:HB3	1.67	0.76
1:B:444:THR:HG22	1:B:447:GLU:HG3	1.69	0.75
1:B:159:LYS:HD3	1:B:164:SER:O	1.87	0.74
1:A:372:ARG:HH12	1:A:445:LEU:HA	1.51	0.73
1:B:444:THR:HG23	1:B:447:GLU:H	1.54	0.72
1:A:484:PHE:CZ	1:B:67:SER:HA	2.26	0.70
1:A:100:ALA:HB2	1:A:266:MET:HE1	1.74	0.70
1:B:481:LEU:HB2	1:B:484:PHE:HB3	1.74	0.69
1:A:159:LYS:HD3	1:A:164:SER:O	1.92	0.69
1:A:275:SER:HB3	1:A:284:ILE:CD1	2.19	0.67
1:A:15:TRP:HD1	1:A:16:SER:N	1.92	0.67
1:A:376:VAL:HB	1:A:432:THR:HG22	1.78	0.66
1:A:408:LEU:HB3	1:A:413:LEU:HG	1.79	0.65
1:A:15:TRP:CD1	1:A:16:SER:N	2.64	0.65
1:A:59:ARG:HG3	1:A:481:LEU:HD23	1.78	0.65
1:A:436:GLN:O	1:A:439:THR:HG22	1.96	0.65
1:A:350:VAL:HG12	1:A:351:THR:HG23	1.79	0.64
1:B:444:THR:HG22	1:B:447:GLU:CG	2.26	0.64
1:A:415:GLU:O	1:A:419:GLN:HG3	1.97	0.64
1:B:336:ARG:HG3	1:B:336:ARG:HH11	1.62	0.63
1:A:75:GLN:HB3	1:A:297:PHE:CZ	2.34	0.63
1:A:336:ARG:HH11	1:A:336:ARG:HG3	1.63	0.63
1:A:453:ALA:HA	1:A:459:GLN:NE2	2.13	0.62
1:B:75:GLN:HB3	1:B:297:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:O	1:B:419:GLN:HG3	2.00	0.62
1:B:143:LEU:HD21	1:B:149:LEU:HD23	1.81	0.61
1:A:372:ARG:NH1	1:A:445:LEU:HA	2.15	0.61
1:A:376:VAL:CB	1:A:432:THR:HG22	2.30	0.61
1:B:446:LYS:O	1:B:450:GLU:HG3	2.01	0.60
1:B:405:THR:N	1:B:406:PRO:CD	2.65	0.60
1:A:438:ASP:HB3	1:A:451:LYS:HE2	1.83	0.60
1:B:59:ARG:HG3	1:B:481:LEU:CD2	2.31	0.60
1:B:100:ALA:HB2	1:B:266:MET:HE1	1.83	0.60
1:B:59:ARG:O	1:B:63:GLU:HG3	2.01	0.59
1:B:282:LYS:HE2	1:B:282:LYS:HA	1.84	0.59
1:A:326:GLU:HG2	1:B:15:TRP:HB3	1.85	0.59
1:B:375:LYS:HG3	1:B:449:LYS:HE2	1.85	0.58
1:A:458:HIS:O	1:A:461:ALA:N	2.36	0.58
1:B:240:VAL:HG11	1:B:332:VAL:HG21	1.85	0.58
1:A:405:THR:N	1:A:406:PRO:CD	2.66	0.58
1:A:54:GLU:OE2	1:B:73:TYR:HB2	2.03	0.58
1:A:386:LYS:HD2	1:A:398:PRO:CG	2.31	0.58
1:B:408:LEU:HB3	1:B:413:LEU:HG	1.86	0.58
1:B:444:THR:CG2	1:B:447:GLU:HG3	2.32	0.58
1:A:73:TYR:HB2	1:B:54:GLU:OE2	2.03	0.58
1:A:139:MET:CE	1:A:195:PRO:HG3	2.34	0.58
1:B:145:ASP:HB3	1:B:174:VAL:HG13	1.86	0.57
1:A:115:VAL:HG12	1:A:266:MET:CE	2.33	0.57
1:B:405:THR:N	1:B:406:PRO:HD3	2.19	0.57
1:B:115:VAL:HG12	1:B:266:MET:CE	2.35	0.57
1:A:143:LEU:HD21	1:A:149:LEU:HD23	1.87	0.57
1:A:145:ASP:HB3	1:A:174:VAL:HG13	1.87	0.56
1:B:240:VAL:CG1	1:B:332:VAL:HG21	2.36	0.56
1:A:139:MET:HG3	1:A:195:PRO:HB3	1.87	0.56
1:B:386:LYS:HD2	1:B:398:PRO:CG	2.35	0.56
1:B:115:VAL:HG12	1:B:266:MET:HE3	1.88	0.56
1:A:137:ARG:HB3	1:A:193:PHE:CE2	2.42	0.55
1:A:326:GLU:HG2	1:B:15:TRP:CB	2.37	0.55
1:A:59:ARG:O	1:A:63:GLU:HG3	2.07	0.55
1:A:405:THR:N	1:A:406:PRO:HD3	2.23	0.54
1:B:59:ARG:HG3	1:B:481:LEU:HD23	1.89	0.54
1:A:455:ASP:HB3	1:A:458:HIS:HB2	1.90	0.54
1:A:116:GLN:N	1:A:117:PRO:CD	2.71	0.53
1:B:148:HIS:HD2	1:B:150:THR:OG1	1.91	0.53
1:B:116:GLN:N	1:B:117:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:SER:HB2	1:A:354:SER:HB2	1.89	0.53
1:B:206:SER:HB2	1:B:354:SER:HB2	1.90	0.53
1:A:132:VAL:O	1:A:133:GLU:HB2	2.09	0.52
1:B:132:VAL:O	1:B:133:GLU:HB2	2.08	0.52
1:B:358:LEU:C	1:B:358:LEU:HD12	2.29	0.52
1:A:357:HIS:H	1:A:357:HIS:HD1	1.56	0.52
1:B:87:GLU:O	1:B:91:GLU:HG3	2.11	0.51
1:A:139:MET:HE2	1:A:195:PRO:HG3	1.92	0.51
1:B:121:SER:HB2	1:B:122:PRO:HD3	1.91	0.51
1:A:148:HIS:HD2	1:A:150:THR:OG1	1.93	0.51
1:A:446:LYS:HA	1:A:449:LYS:HG2	1.93	0.51
1:B:413:LEU:HD13	1:B:417:ASP:CB	2.40	0.51
1:A:115:VAL:HG12	1:A:266:MET:HE2	1.93	0.51
1:B:235:LEU:HA	1:B:328:GLN:HG2	1.93	0.50
1:B:319:ALA:HA	1:B:324:PHE:CG	2.47	0.50
1:A:231:HIS:HD2	1:A:357:HIS:NE2	2.09	0.50
1:B:139:MET:CE	1:B:195:PRO:HG3	2.41	0.50
1:A:240:VAL:CG1	1:A:332:VAL:HG21	2.42	0.50
1:A:240:VAL:HG11	1:A:332:VAL:HG21	1.92	0.50
1:B:369:ASP:HB2	1:B:398:PRO:O	2.11	0.50
1:A:319:ALA:HA	1:A:324:PHE:CG	2.47	0.50
1:B:211:TYR:CZ	1:B:244:PRO:HB3	2.47	0.50
1:B:231:HIS:HD2	1:B:357:HIS:NE2	2.10	0.49
1:A:455:ASP:OD1	1:A:457:LYS:HG2	2.11	0.49
1:B:357:HIS:H	1:B:357:HIS:HD1	1.61	0.49
1:A:369:ASP:HB2	1:A:398:PRO:O	2.13	0.49
1:A:433:VAL:O	1:A:436:GLN:HB3	2.12	0.49
1:B:413:LEU:HD22	1:B:476:PHE:CE2	2.48	0.49
1:B:427:ARG:HH22	1:B:468:GLU:CD	2.15	0.49
1:A:50:LEU:HB2	1:A:383:ALA:O	2.13	0.48
1:A:87:GLU:O	1:A:91:GLU:HG3	2.14	0.48
1:A:457:LYS:N	1:A:457:LYS:HD3	2.29	0.48
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.79	0.48
1:A:211:TYR:CZ	1:A:244:PRO:HB3	2.49	0.48
1:B:405:THR:H	1:B:406:PRO:HD3	1.78	0.47
1:A:119:SER:C	1:A:122:PRO:HD2	2.35	0.47
1:A:275:SER:O	1:A:284:ILE:HG12	2.15	0.47
1:A:436:GLN:HA	1:A:439:THR:HG22	1.96	0.47
1:B:137:ARG:HB3	1:B:193:PHE:CE2	2.48	0.47
1:A:174:VAL:HA	1:A:181:ILE:HA	1.96	0.47
1:B:350:VAL:HG12	1:B:351:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:C	1:A:358:LEU:HD12	2.35	0.46
1:B:350:VAL:HG21	1:B:360:LEU:HD23	1.97	0.46
1:A:115:VAL:HG12	1:A:266:MET:HE3	1.96	0.46
1:A:427:ARG:HH22	1:A:468:GLU:CD	2.19	0.46
1:B:139:MET:HG3	1:B:195:PRO:HB3	1.97	0.46
1:B:148:HIS:CD2	1:B:150:THR:H	2.34	0.46
1:B:481:LEU:O	1:B:483:GLY:N	2.48	0.46
1:B:143:LEU:HD22	1:B:153:PHE:CD1	2.50	0.46
1:A:446:LYS:O	1:A:450:GLU:HG3	2.16	0.46
1:A:367:GLY:O	1:A:436:GLN:NE2	2.49	0.45
1:A:148:HIS:CD2	1:A:150:THR:H	2.34	0.45
1:B:336:ARG:HG3	1:B:336:ARG:NH1	2.29	0.45
1:B:37:ILE:HG21	1:B:484:PHE:CE1	2.52	0.45
1:A:380:CYS:SG	1:A:465:LEU:HD23	2.56	0.45
1:A:405:THR:H	1:A:406:PRO:HD3	1.81	0.45
1:A:361:VAL:O	1:A:400:GLY:HA2	2.17	0.45
1:A:22:LEU:HA	1:B:58:SER:HB2	1.99	0.45
1:A:126:ALA:HA	1:A:300:LEU:CD1	2.47	0.45
1:A:466:ARG:O	1:A:470:GLU:HG3	2.17	0.44
1:B:393:LYS:N	1:B:393:LYS:HD2	2.32	0.44
1:B:77:TYR:HB3	1:B:78:PRO:HD2	1.99	0.44
1:B:372:ARG:HB3	1:B:448:PHE:CZ	2.53	0.44
1:A:336:ARG:HG3	1:A:336:ARG:NH1	2.31	0.44
1:B:184:ASP:OD1	1:B:213:ARG:NH2	2.51	0.44
1:A:179:GLY:HA3	1:A:351:THR:HG22	1.98	0.44
1:A:458:HIS:C	1:A:460:ARG:N	2.68	0.44
1:A:121:SER:HB2	1:A:122:PRO:HD3	1.99	0.44
1:B:361:VAL:O	1:B:400:GLY:HA2	2.18	0.44
1:A:206:SER:HB2	1:A:354:SER:CB	2.47	0.44
1:A:327:TYR:HB2	1:B:18:HIS:CD2	2.53	0.44
1:B:139:MET:HE2	1:B:195:PRO:HG3	1.99	0.43
1:B:100:ALA:HB2	1:B:266:MET:CE	2.48	0.43
1:B:119:SER:C	1:B:122:PRO:HD2	2.38	0.43
1:B:466:ARG:O	1:B:470:GLU:HG3	2.17	0.43
1:A:24:GLN:HA	1:A:25:PRO:HD3	1.87	0.43
1:A:393:LYS:N	1:A:393:LYS:HD2	2.34	0.43
1:A:396:LEU:HD22	1:A:396:LEU:N	2.33	0.43
1:A:413:LEU:HD22	1:A:476:PHE:CE2	2.54	0.43
1:A:17:SER:HA	1:A:20:GLN:HG3	2.01	0.43
1:A:456:GLU:O	1:A:460:ARG:HB2	2.19	0.42
1:B:224:TYR:CE1	1:B:288:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:HE1	1:A:195:PRO:HG3	2.01	0.42
1:B:50:LEU:HB2	1:B:383:ALA:O	2.19	0.42
1:B:271:ARG:HD3	1:B:289:GLU:OE1	2.18	0.42
1:A:446:LYS:HD3	1:A:446:LYS:C	2.40	0.42
1:B:140:GLY:O	1:B:171:ALA:HA	2.20	0.42
1:A:227:ALA:HB2	1:A:248:CYS:SG	2.59	0.42
1:A:457:LYS:HD3	1:A:457:LYS:H	1.84	0.42
1:B:238:ALA:HA	1:B:325:LYS:HD3	2.01	0.42
1:B:266:MET:HE1	1:B:316:LEU:HD11	2.01	0.42
1:B:275:SER:O	1:B:283:GLU:HB2	2.20	0.42
1:A:17:SER:HA	1:A:20:GLN:CG	2.50	0.42
1:A:184:ASP:OD1	1:A:213:ARG:NH2	2.53	0.42
1:A:143:LEU:HD22	1:A:153:PHE:CD1	2.54	0.42
1:B:45:ARG:HB2	1:B:478:LEU:HD22	2.02	0.42
1:A:71:ASN:HD21	1:B:57:ALA:H	1.68	0.42
1:A:435:ILE:CD1	1:A:452:LEU:HD13	2.49	0.42
1:B:413:LEU:HD22	1:B:476:PHE:CD2	2.55	0.42
1:B:444:THR:CG2	1:B:447:GLU:H	2.28	0.42
1:A:139:MET:HE1	1:A:190:ALA:HA	2.02	0.41
1:A:93:GLU:O	1:A:97:GLN:HG3	2.20	0.41
1:A:224:TYR:CE1	1:A:288:LEU:HD21	2.55	0.41
1:A:140:GLY:O	1:A:171:ALA:HA	2.21	0.41
1:A:233:SER:O	1:A:237:VAL:HG23	2.19	0.41
1:B:396:LEU:HD22	1:B:396:LEU:N	2.35	0.41
1:A:62:LEU:HD13	1:B:66:GLY:O	2.21	0.41
1:A:235:LEU:HA	1:A:328:GLN:HG2	2.02	0.41
1:B:116:GLN:N	1:B:117:PRO:HD3	2.35	0.41
1:B:227:ALA:HB2	1:B:248:CYS:SG	2.60	0.41
1:B:80:GLN:HG2	1:B:80:GLN:O	2.21	0.41
1:B:93:GLU:O	1:B:97:GLN:HG3	2.21	0.41
1:B:174:VAL:HA	1:B:181:ILE:HA	2.01	0.41
1:B:206:SER:HB2	1:B:354:SER:CB	2.51	0.41
1:A:132:VAL:HG12	1:A:136:GLY:HA3	2.01	0.41
1:A:145:ASP:OD2	1:A:173:LYS:HB3	2.21	0.41
1:B:274:ARG:HG3	1:B:286:TYR:CZ	2.56	0.41
1:A:240:VAL:CG1	1:A:240:VAL:O	2.68	0.41
1:B:240:VAL:HG11	1:B:332:VAL:CG2	2.50	0.40
1:A:116:GLN:N	1:A:117:PRO:HD3	2.35	0.40
1:A:484:PHE:HZ	1:B:67:SER:HA	1.82	0.40
1:B:24:GLN:HA	1:B:25:PRO:HD3	1.98	0.40
1:A:479:PRO:CG	1:B:22:LEU:HD13	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:HE2	3:B:601:PO4:O4	2.21	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	459/483 (95%)	432 (94%)	25 (5%)	2 (0%)	34	54
1	B	462/483 (96%)	435 (94%)	24 (5%)	3 (1%)	25	43
All	All	921/966 (95%)	867 (94%)	49 (5%)	5 (0%)	29	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	ASP
1	A	482	PRO
1	B	392	ASP
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	378/391 (97%)	367 (97%)	11 (3%)	42 69
1	B	381/391 (97%)	373 (98%)	8 (2%)	53 78
All	All	759/782 (97%)	740 (98%)	19 (2%)	47 73

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	73	TYR
1	A	119	SER
1	A	215	ARG
1	A	231	HIS
1	A	305	HIS
1	A	387	ASN
1	A	413	LEU
1	A	442	ARG
1	A	446	LYS
1	A	482	PRO
1	B	73	TYR
1	B	119	SER
1	B	215	ARG
1	B	231	HIS
1	B	283	GLU
1	B	387	ASN
1	B	413	LEU
1	B	434	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	387	ASN
1	A	459	GLN

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Mol	Chain	Res	Type
1	A	467	GLN
1	B	71	ASN
1	B	102	GLN
1	B	109	GLN
1	B	148	HIS
1	B	231	HIS
1	B	287	ASN
1	B	305	HIS
1	B	387	ASN
1	B	459	GLN
1	B	467	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	PLP	B	600	1	15,15,16	4.79	10 (66%)	20,22,23	2.95	7 (35%)
2	PLP	A	500	1	15,15,16	4.93	10 (66%)	20,22,23	2.96	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	B	601	-	4,4,4	1.66	1 (25%)	6,6,6	0.44	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
2	PLP	B	600	1	-	0/6/6/8	0/1/1/1
2	PLP	A	500	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)
2	B	600	PLP	C4A-C4	-9.25	1.32	1.51
2	A	500	PLP	C3-C2	8.99	1.49	1.40
2	A	500	PLP	C4A-C4	-8.72	1.33	1.51
2	B	600	PLP	C3-C2	8.08	1.49	1.40
2	A	500	PLP	C5-C4	8.02	1.49	1.40
2	A	500	PLP	C3-C4	6.97	1.54	1.40
2	B	600	PLP	C5-C4	6.88	1.48	1.40
2	B	600	PLP	C3-C4	6.66	1.54	1.40
2	B	600	PLP	P-O4P	-5.39	1.42	1.60
2	A	500	PLP	P-O4P	-5.19	1.43	1.60
2	B	600	PLP	C6-C5	4.39	1.46	1.37
2	B	600	PLP	C2-N1	4.33	1.42	1.33
2	A	500	PLP	C2-N1	4.08	1.41	1.33
2	A	500	PLP	C6-C5	4.07	1.46	1.37
2	A	500	PLP	P-O3P	-3.88	1.39	1.54
2	B	600	PLP	P-O3P	-3.80	1.40	1.54
2	B	600	PLP	P-O2P	-3.05	1.43	1.54
2	A	500	PLP	P-O2P	-2.88	1.43	1.54
2	A	500	PLP	C6-N1	2.82	1.40	1.34
2	B	600	PLP	C6-N1	2.68	1.40	1.34
3	B	601	PO4	P-O4	-2.08	1.48	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	PLP	O3P-P-O4P	7.80	127.48	106.73
2	A	500	PLP	O3P-P-O4P	7.64	127.06	106.73
2	A	500	PLP	O4P-C5A-C5	7.49	123.62	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	PLP	O4P-C5A-C5	7.13	122.94	109.35
2	A	500	PLP	C6-N1-C2	3.92	126.43	119.17
2	B	600	PLP	C6-N1-C2	3.76	126.13	119.17
2	A	500	PLP	O3-C3-C2	3.56	125.26	117.49
2	B	600	PLP	O3-C3-C2	3.49	125.09	117.49
2	B	600	PLP	C4A-C4-C5	-3.22	117.62	120.94
2	A	500	PLP	C4A-C4-C5	-2.64	118.21	120.94
2	B	600	PLP	C5-C6-N1	-2.63	119.43	123.82
2	A	500	PLP	C5-C6-N1	-2.39	119.83	123.82
2	A	500	PLP	O3P-P-O1P	-2.20	102.08	110.68
2	A	500	PLP	C3-C2-N1	-2.17	117.96	120.77
2	B	600	PLP	O3P-P-O1P	-2.12	102.38	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	PO4	1	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%)	-0.02	23 (4%) 28 30	15, 32, 78, 124	0
1	B	466/483 (96%)	-0.18	15 (3%) 47 51	15, 30, 76, 132	0
All	All	929/966 (96%)	-0.10	38 (4%) 37 40	15, 31, 78, 132	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	PHE	5.7
1	B	284	ILE	5.6
1	B	275	SER	5.1
1	A	459	GLN	4.9
1	B	276	VAL	4.7
1	A	435	ILE	4.5
1	B	15	TRP	4.5
1	A	284	ILE	4.4
1	A	483	GLY	4.3
1	A	484	PHE	4.3
1	B	273	VAL	4.1
1	A	285	LEU	4.1
1	B	282	LYS	4.1
1	B	283	GLU	4.0
1	A	16	SER	3.8
1	B	483	GLY	3.6
1	A	283	GLU	3.6
1	A	275	SER	3.6
1	B	277	ASP	3.3
1	B	442	ARG	3.3
1	A	432	THR	3.3
1	A	441	PRO	3.1
1	B	16	SER	2.9
1	A	273	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	475	LEU	2.8
1	A	448	PHE	2.7
1	A	462	VAL	2.6
1	A	452	LEU	2.6
1	A	272	GLY	2.6
1	A	439	THR	2.5
1	A	463	ARG	2.4
1	A	461	ALA	2.3
1	B	393	LYS	2.3
1	A	15	TRP	2.2
1	A	449	LYS	2.1
1	B	17	SER	2.0
1	B	396	LEU	2.0
1	A	446	LYS	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(Å <sup>2</sup> )	Q<0.9
3	PO4	B	601	5/5	0.91	0.23	74,74,76,76	0
2	PLP	B	600	15/16	0.96	0.16	27,30,32,34	0
2	PLP	A	500	15/16	0.96	0.15	23,26,29,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.