



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:15 pm GMT

PDB ID : 1VA6  
Title : Crystal structure of Gamma-glutamylcysteine synthetase from Escherichia Coli B complexed with Transition-state analogue  
Authors : Hibi, T.; Nii, H.; Nakatsu, T.; Kato, H.; Hiratake, J.; Oda, J.  
Deposited on : 2004-02-12  
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

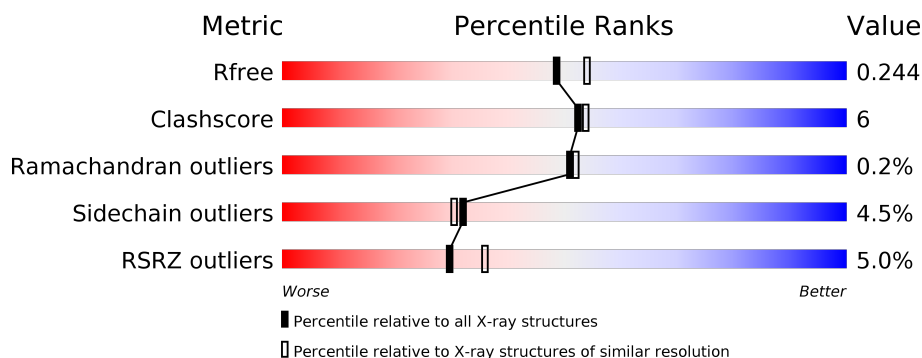
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	518	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
1	B	518	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8486 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 Glutamate–cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4017	2549	685	765	18			
1	B	503	Total	C	N	O	S	0	0	0
			3981	2528	679	756	18			

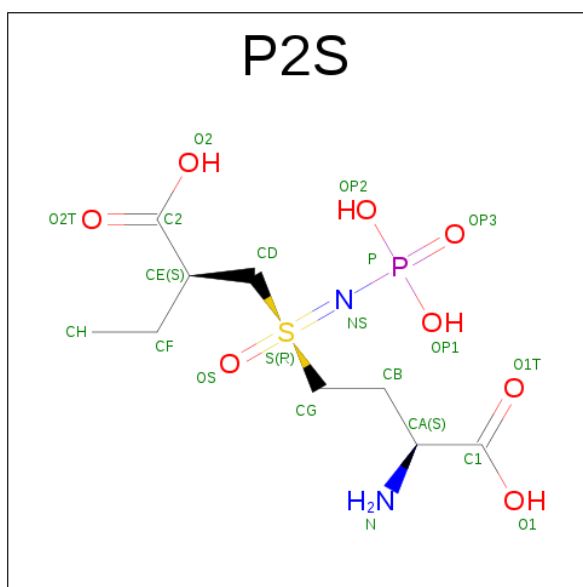
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	CYS	ENGINEERED	UNP P0A6W9
A	164	SER	CYS	ENGINEERED	UNP P0A6W9
A	205	SER	CYS	ENGINEERED	UNP P0A6W9
A	223	SER	CYS	ENGINEERED	UNP P0A6W9
B	106	SER	CYS	ENGINEERED	UNP P0A6W9
B	164	SER	CYS	ENGINEERED	UNP P0A6W9
B	205	SER	CYS	ENGINEERED	UNP P0A6W9
B	223	SER	CYS	ENGINEERED	UNP P0A6W9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

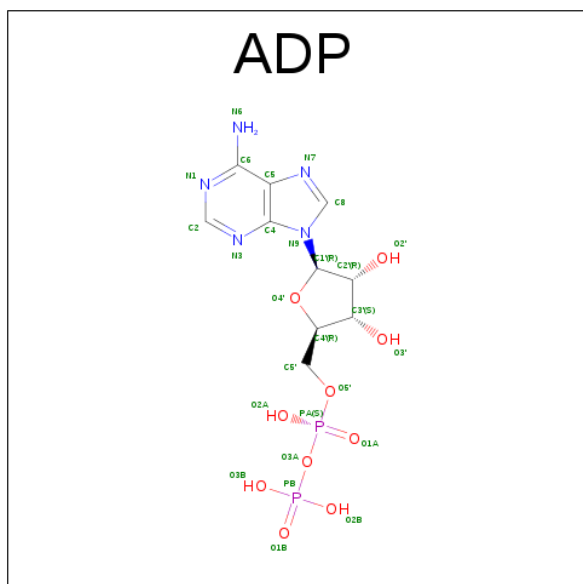
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Mg	0	0
			4	4		
2	A	4	Total	Mg	0	0
			4	4		

- Molecule 3 is (2S)-2-AMINO-4-[[[(2R)-2-CARBOXYBUTYL](PHOSPHONO)SULFONIMIDOYL]BUTANOIC ACID (three-letter code: P2S) (formula: C<sub>9</sub>H<sub>19</sub>N<sub>2</sub>O<sub>8</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	N 2	O 8	P 1	S 1	0	0
3	B	1	Total 21	C 9	N 2	O 8	P 1	S 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



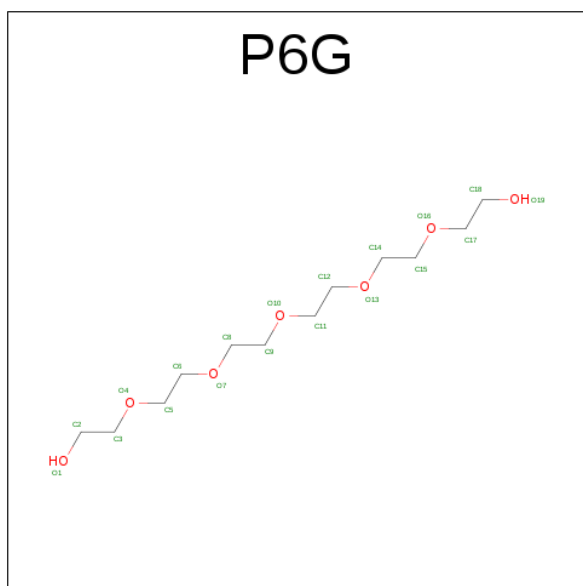
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		
5	B	1	Total	C	O	0	0
			19	12	7		

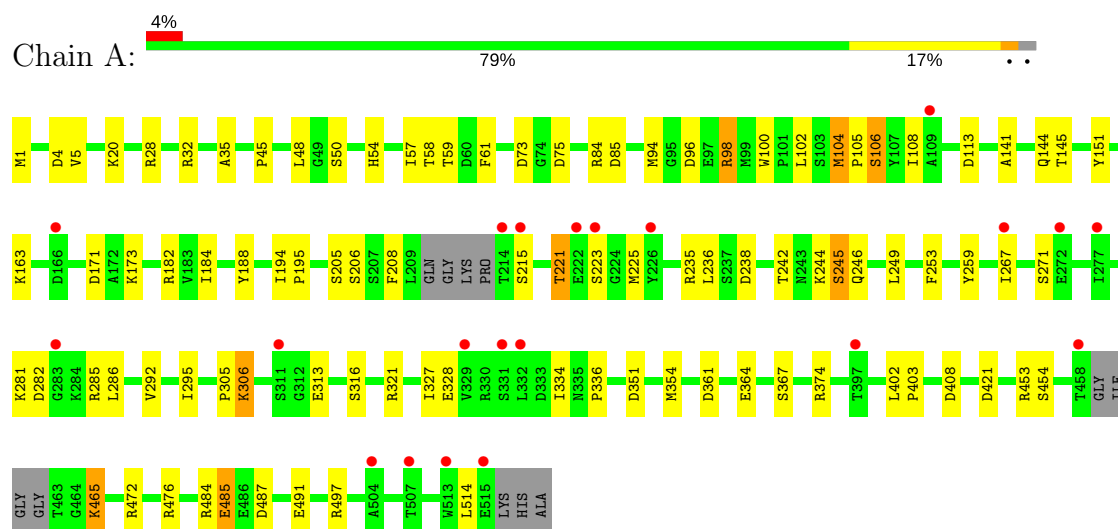
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	194	Total	O	0	0
			194	194		
6	B	152	Total	O	0	0
			152	152		

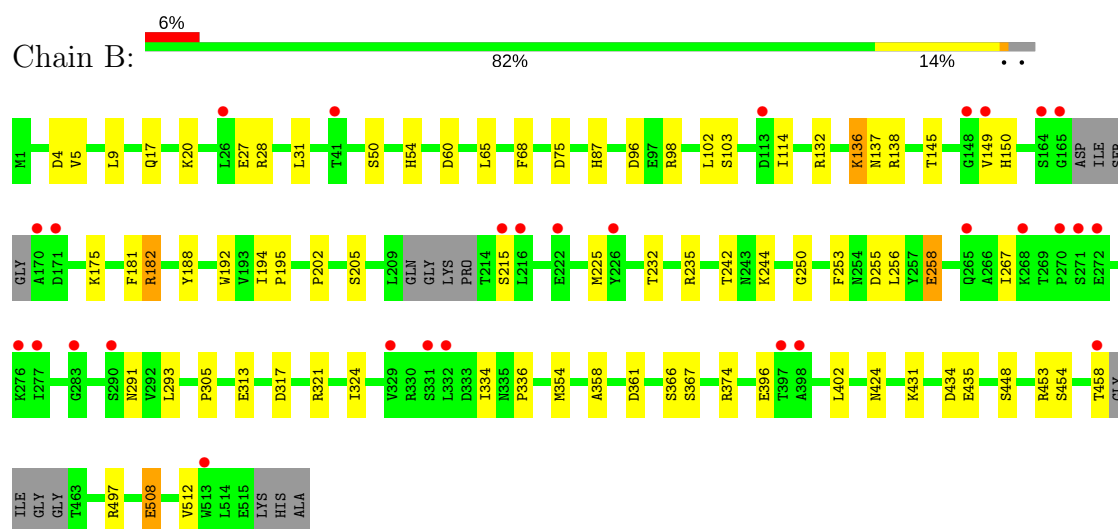
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: Glutamate–cysteine ligase



#### • Molecule 1: Glutamate–cysteine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.47Å 97.36Å 102.19Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-2.10) 97.0 (39.25-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.200 , 0.225 0.226 , 0.244	Depositor DCC
$R_{free}$ test set	3701 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P2S, MG, ADP, P6G

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	0.86	0/4103	0.80	13/5555 (0.2%)
1	B	0.77	0/4066	0.79	7/5506 (0.1%)
All	All	0.82	0/8169	0.80	20/11061 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASP	CB-CG-OD2	7.87	125.38	118.30
1	A	282	ASP	CB-CG-OD2	7.20	124.78	118.30
1	B	96	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	96	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	60	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	4	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	361	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	408	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	487	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	73	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	317	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	113	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	421	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	85	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	238	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	4	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	75	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	361	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	434	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	171	ASP	CB-CG-OD2	5.01	122.81	118.30

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	4017	0	3935	56	0
1	B	3981	0	3889	44	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	21	0	15	0	0
3	B	21	0	15	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	19	0	26	5	0
5	B	19	0	26	7	0
6	A	194	0	0	6	0
6	B	152	0	0	4	0
All	All	8486	0	7930	101	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 6.

All (101) 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:431:LYS:HE2	1:B:435:GLU:OE2	1.79	0.82
1:A:242:THR:HG22	1:A:244:LYS:H	1.47	0.77
1:A:205:SER:HA	1:A:225:MET:HE2	1.67	0.76
1:A:188:TYR:HE1	5:A:526:P6G:H152	1.54	0.72
1:A:485:GLU:HG2	6:A:678:HOH:O	1.90	0.70
1:B:188:TYR:HE1	5:B:1526:P6G:H152	1.57	0.69
1:B:508:GLU:HG2	6:B:1674:HOH:O	1.92	0.69
1:A:305:PRO:O	1:A:306:LYS:HG2	1.94	0.68
1:B:192:TRP:O	1:B:195:PRO:HD2	1.93	0.67
1:A:497:ARG:HD2	6:A:677:HOH:O	1.97	0.65
1:A:5:VAL:HG12	1:A:5:VAL:O	1.97	0.65
1:B:27:GLU:HB2	1:B:150:HIS:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:CD2	5:A:526:P6G:H32	2.28	0.63
1:A:221:THR:HG23	1:A:223:SER:H	1.63	0.63
1:A:1:MET:HE3	6:A:577:HOH:O	1.98	0.63
1:A:100:TRP:CZ2	1:A:106:SER:HB2	2.34	0.62
1:B:242:THR:HG22	1:B:244:LYS:H	1.64	0.62
1:A:285:ARG:NH1	1:A:514:LEU:HD12	2.16	0.60
1:B:194:ILE:HB	1:B:195:PRO:HD3	1.84	0.60
1:B:374:ARG:HD2	5:B:1526:P6G:H141	1.85	0.59
1:A:163:LYS:HE2	6:A:643:HOH:O	2.02	0.58
1:B:114:ILE:HD13	1:B:145:THR:HG21	1.84	0.58
1:B:374:ARG:HB2	5:B:1526:P6G:H142	1.85	0.58
1:B:192:TRP:C	1:B:195:PRO:HD2	2.24	0.58
1:A:334:ILE:O	1:A:336:PRO:HD3	2.03	0.58
1:A:259:TYR:CZ	1:A:305:PRO:HG2	2.40	0.57
1:B:267:ILE:HD13	1:B:293:LEU:HB2	1.86	0.57
1:B:235:ARG:NH2	5:B:1526:P6G:H22	2.19	0.56
5:B:1526:P6G:H32	6:B:1633:HOH:O	2.04	0.56
1:A:281:LYS:HB3	1:A:286:LEU:HD11	1.87	0.56
1:A:141:ALA:O	1:A:145:THR:HG23	2.06	0.55
1:A:105:PRO:HD2	1:A:208:PHE:CZ	2.42	0.55
1:A:151:TYR:OH	1:A:351:ASP:OD1	2.23	0.55
1:B:188:TYR:CE1	5:B:1526:P6G:H152	2.40	0.54
1:A:54:HIS:HB3	1:A:57:ILE:O	2.09	0.53
1:B:68:PHE:CD2	1:B:87:HIS:CE1	2.97	0.52
1:A:32:ARG:HG2	1:A:94:MET:CE	2.39	0.52
1:B:242:THR:HG22	1:B:244:LYS:N	2.25	0.52
1:A:259:TYR:CE2	1:A:305:PRO:HG2	2.45	0.52
1:A:45:PRO:HD2	1:A:48:LEU:HD12	1.90	0.51
1:B:305:PRO:HB3	1:B:324:ILE:HD13	1.92	0.51
1:A:313:GLU:OE1	1:A:321:ARG:NH1	2.43	0.51
1:A:364:GLU:HG3	6:A:691:HOH:O	2.11	0.50
1:B:17:GLN:HB2	6:B:1672:HOH:O	2.11	0.50
1:B:181:PHE:CE2	1:B:256:LEU:HA	2.47	0.50
1:A:267:ILE:HD12	1:A:295:ILE:HA	1.95	0.49
1:B:454:SER:O	1:B:458:THR:HG23	2.13	0.49
1:B:334:ILE:O	1:B:336:PRO:HD3	2.13	0.48
1:A:50:SER:O	1:A:54:HIS:HB2	2.14	0.48
1:A:306:LYS:NZ	1:A:328:GLU:OE1	2.42	0.48
1:B:225:MET:HE2	1:B:225:MET:HA	1.94	0.47
1:B:202:PRO:HD2	6:B:1601:HOH:O	2.13	0.47
1:B:402:LEU:C	1:B:402:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:OH	1:A:305:PRO:HD2	2.15	0.47
1:B:374:ARG:HD2	5:B:1526:P6G:C14	2.45	0.47
1:A:244:LYS:C	1:A:246:GLN:H	2.19	0.47
1:B:313:GLU:OE1	1:B:321:ARG:NH1	2.48	0.47
1:A:472:ARG:O	1:A:476:ARG:HG3	2.15	0.47
1:B:132:ARG:HH11	1:B:132:ARG:HG3	1.80	0.46
1:A:61:PHE:CG	1:A:144:GLN:HB3	2.49	0.46
1:A:102:LEU:HD23	1:A:336:PRO:HB3	1.98	0.46
1:B:181:PHE:HE2	1:B:256:LEU:HA	1.81	0.46
1:B:431:LYS:HE2	1:B:435:GLU:CD	2.35	0.46
1:B:255:ASP:HB3	1:B:258:GLU:HB2	1.98	0.45
1:A:188:TYR:CE1	5:A:526:P6G:H152	2.44	0.45
1:A:244:LYS:C	1:A:246:GLN:N	2.70	0.45
1:A:104:MET:HE1	1:A:235:ARG:HA	1.98	0.44
1:B:102:LEU:HD23	1:B:336:PRO:HB3	2.00	0.44
1:B:138:ARG:NH2	1:B:291:ASN:O	2.43	0.44
1:A:184:ILE:HG21	1:A:253:PHE:CD1	2.52	0.44
1:A:32:ARG:HG2	1:A:94:MET:HE1	2.00	0.44
1:B:5:VAL:HB	1:B:9:LEU:HD12	1.99	0.44
1:A:305:PRO:O	1:A:306:LYS:CG	2.64	0.44
1:A:105:PRO:HB3	1:A:108:ILE:HD12	1.99	0.44
1:A:182:ARG:NH1	6:A:666:HOH:O	2.51	0.44
1:A:105:PRO:HD2	1:A:208:PHE:HZ	1.83	0.44
1:A:54:HIS:NE2	1:A:491:GLU:HG3	2.33	0.43
1:B:50:SER:O	1:B:54:HIS:HB2	2.18	0.43
1:A:465:LYS:HE2	1:A:465:LYS:HB3	1.78	0.43
1:B:149:VAL:HG23	1:B:334:ILE:HD13	2.00	0.43
1:B:225:MET:HA	1:B:225:MET:CE	2.48	0.43
1:A:249:LEU:HD21	1:A:292:VAL:HG11	2.01	0.42
1:A:514:LEU:HA	1:A:514:LEU:HD23	1.91	0.42
1:A:35:ALA:HA	1:A:98:ARG:HD3	2.01	0.42
1:B:250:GLY:HA2	1:B:367:SER:OG	2.19	0.42
1:B:232:THR:HA	1:B:448:SER:CB	2.49	0.42
1:A:194:ILE:HB	1:A:195:PRO:CD	2.50	0.42
1:A:194:ILE:HB	1:A:195:PRO:HD3	2.02	0.42
1:A:402:LEU:N	1:A:403:PRO:CD	2.83	0.42
1:B:31:LEU:CD2	1:B:65:LEU:HD13	2.51	0.41
1:A:104:MET:CE	1:A:235:ARG:HA	2.50	0.41
1:A:374:ARG:HG3	5:A:526:P6G:H121	2.03	0.41
1:A:402:LEU:HD23	1:A:402:LEU:C	2.41	0.41
1:B:136:LYS:HG2	1:B:137:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HD23	5:A:526:P6G:H32	2.03	0.41
1:B:188:TYR:CE2	1:B:253:PHE:CE2	3.09	0.41
1:B:182:ARG:HD2	1:B:182:ARG:HH11	1.76	0.40
1:B:205:SER:HA	1:B:225:MET:HE2	2.03	0.40
1:B:182:ARG:HD3	1:B:358:ALA:O	2.20	0.40
1:A:244:LYS:O	1:A:246:GLN:N	2.55	0.40
1:A:58:THR:OG1	1:A:59:THR:N	2.53	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	501/518 (97%)	489 (98%)	11 (2%)	1 (0%)	51	52
1	B	495/518 (96%)	480 (97%)	14 (3%)	1 (0%)	51	52
All	All	996/1036 (96%)	969 (97%)	25 (2%)	2 (0%)	51	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLU
1	A	245	SER

### 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	424/434 (98%)	402 (95%)	22 (5%)	27	24
1	B	418/434 (96%)	402 (96%)	16 (4%)	38	38
All	All	842/868 (97%)	804 (96%)	38 (4%)	32	30

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	28	ARG
1	A	84	ARG
1	A	98	ARG
1	A	104	MET
1	A	106	SER
1	A	173	LYS
1	A	206	SER
1	A	215	SER
1	A	221	THR
1	A	245	SER
1	A	271	SER
1	A	306	LYS
1	A	316	SER
1	A	327	ILE
1	A	354	MET
1	A	367	SER
1	A	453	ARG
1	A	454	SER
1	A	465	LYS
1	A	484	ARG
1	A	485	GLU
1	B	20	LYS
1	B	28	ARG
1	B	98	ARG
1	B	103	SER
1	B	136	LYS
1	B	175	LYS
1	B	182	ARG
1	B	215	SER
1	B	258	GLU
1	B	354	MET
1	B	366	SER
1	B	424	ASN
1	B	453	ARG

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Mol	Chain	Res	Type
1	B	497	ARG
1	B	508	GLU
1	B	512	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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	P2S	A	520	2	10,20,20	4.55	6 (60%)	9,29,29	1.83	3 (33%)
4	ADP	A	521	2	25,29,29	1.28	4 (16%)	24,45,45	2.24	3 (12%)
5	P6G	A	526	-	18,18,18	0.58	0	17,17,17	0.77	0
3	P2S	B	1520	2	10,20,20	4.25	6 (60%)	9,29,29	1.56	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ADP	B	1521	2	25,29,29	1.08	1 (4%)	24,45,45	2.27	6 (25%)
5	P6G	B	1526	-	18,18,18	0.64	0	17,17,17	0.83	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	P2S	A	520	2	-	0/11/27/27	0/0/0/0
4	ADP	A	521	2	-	0/12/32/32	0/3/3/3
5	P6G	A	526	-	-	0/16/16/16	0/0/0/0
3	P2S	B	1520	2	-	0/11/27/27	0/0/0/0
4	ADP	B	1521	2	-	0/12/32/32	0/3/3/3
5	P6G	B	1526	-	-	0/16/16/16	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1520	P2S	CB-CG	-8.75	1.43	1.52
3	A	520	P2S	CG-S	-7.71	1.70	1.79
3	A	520	P2S	CB-CG	-7.38	1.44	1.52
3	B	1520	P2S	CG-S	-5.72	1.72	1.79
3	B	1520	P2S	CF-CE	-3.42	1.41	1.54
3	A	520	P2S	CF-CE	-3.03	1.43	1.54
4	A	521	ADP	O4'-C4'	-2.75	1.38	1.45
4	B	1521	ADP	O4'-C4'	-2.55	1.39	1.45
4	A	521	ADP	C2'-C1'	-2.33	1.49	1.53
4	A	521	ADP	PB-O1B	-2.09	1.43	1.50
3	A	520	P2S	OS-S	2.03	1.58	1.45
4	A	521	ADP	C2-N3	2.31	1.36	1.32
3	B	1520	P2S	P-OP2	2.64	1.60	1.54
3	B	1520	P2S	P-NS	2.81	1.70	1.59
3	A	520	P2S	P-OP2	5.85	1.66	1.54
3	B	1520	P2S	P-OP3	6.00	1.56	1.46
3	A	520	P2S	P-OP3	6.32	1.56	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	521	ADP	N3-C2-N1	-9.10	120.93	128.86
4	B	1521	ADP	N3-C2-N1	-8.95	121.07	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	520	P2S	CF-CE-C2	-3.60	106.64	112.63
4	B	1521	ADP	C5'-C4'-C3'	-2.48	105.85	115.29
3	B	1520	P2S	CF-CE-C2	-2.31	108.78	112.63
3	A	520	P2S	CH-CF-CE	-2.29	107.59	114.19
4	B	1521	ADP	O3'-C3'-C4'	-2.24	104.53	111.09
4	B	1521	ADP	C4'-O4'-C1'	2.05	111.95	109.77
4	A	521	ADP	O4'-C4'-C5'	2.05	116.32	109.40
3	A	520	P2S	OS-S-CG	2.59	113.29	108.63
4	B	1521	ADP	O4'-C4'-C5'	2.62	118.23	109.40
3	B	1520	P2S	OS-S-CG	3.19	114.37	108.63
4	B	1521	ADP	C2'-C3'-C4'	3.34	109.13	102.62
4	A	521	ADP	C2'-C3'-C4'	3.56	109.54	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	526	P6G	5	0
5	B	1526	P6G	7	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	507/518 (97%)	0.16	21 (4%) 38 45	7, 23, 53, 84	0
1	B	503/518 (97%)	0.34	29 (5%) 24 30	9, 28, 63, 93	0
All	All	1010/1036 (97%)	0.25	50 (4%) 30 36	7, 26, 60, 93	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	ALA	5.3
1	B	397	THR	4.6
1	A	311	SER	4.3
1	A	513	TRP	4.1
1	A	222	GLU	4.1
1	B	272	GLU	4.0
1	A	215	SER	4.0
1	B	215	SER	3.9
1	B	171	ASP	3.8
1	B	277	ILE	3.6
1	A	507	THR	3.3
1	B	222	GLU	3.2
1	A	226	TYR	3.1
1	A	515	GLU	3.0
1	B	148	GLY	3.0
1	A	329	VAL	2.9
1	B	398	ALA	2.9
1	B	41	THR	2.9
1	B	283	GLY	2.8
1	A	223	SER	2.8
1	B	290	SER	2.8
1	A	283	GLY	2.8
1	B	26	LEU	2.8
1	A	331	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	397	THR	2.7
1	A	332	LEU	2.6
1	B	164	SER	2.6
1	B	226	TYR	2.6
1	B	270	PRO	2.6
1	B	268	LYS	2.5
1	B	332	LEU	2.5
1	B	458	THR	2.5
1	B	329	VAL	2.5
1	B	149	VAL	2.4
1	A	166	ASP	2.4
1	B	271	SER	2.3
1	A	267	ILE	2.3
1	A	109	ALA	2.2
1	B	165	GLY	2.2
1	B	276	LYS	2.2
1	B	331	SER	2.2
1	A	272	GLU	2.1
1	A	504	ALA	2.1
1	B	265	GLN	2.1
1	A	277	ILE	2.1
1	B	513	TRP	2.1
1	B	113	ASP	2.0
1	B	216	LEU	2.0
1	A	458	THR	2.0
1	A	214	THR	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<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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	P6G	A	526	19/19	0.90	0.23	1.89	27,34,45,45	0
5	P6G	B	1526	19/19	0.83	0.22	1.44	29,34,48,49	0
2	MG	A	523	1/1	0.94	0.22	1.35	15,15,15,15	0
3	P2S	A	520	21/21	0.97	0.17	0.04	9,16,24,26	0
3	P2S	B	1520	21/21	0.96	0.17	-0.13	12,18,26,28	0
4	ADP	B	1521	27/27	0.96	0.16	-0.21	7,11,16,18	0
2	MG	B	1523	1/1	0.81	0.21	-0.31	11,11,11,11	0
4	ADP	A	521	27/27	0.97	0.13	-0.37	3,11,15,18	0
2	MG	B	1525	1/1	0.89	0.06	-1.58	31,31,31,31	0
2	MG	A	525	1/1	0.96	0.03	-2.62	14,14,14,14	0
2	MG	B	1524	1/1	0.94	0.18	-	15,15,15,15	0
2	MG	B	1522	1/1	0.86	0.22	-	21,21,21,21	0
2	MG	A	524	1/1	0.89	0.13	-	14,14,14,14	0
2	MG	A	522	1/1	0.95	0.12	-	18,18,18,18	0

## 6.5 Other polymers

There are no such residues in this entry.