



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2016 – 04:52 PM EDT

PDB ID : 5G0A  
Title : The crystal structure of a S-selective transaminase from *Bacillus megaterium*  
Authors : van Oosterwijk, N.; Willies, S.; Hekelaar, J.; Terwisscha van Scheltinga, A.C.;  
Turner, N.J.; Dijkstra, B.W.  
Deposited on : 2016-03-17  
Resolution : 1.70 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

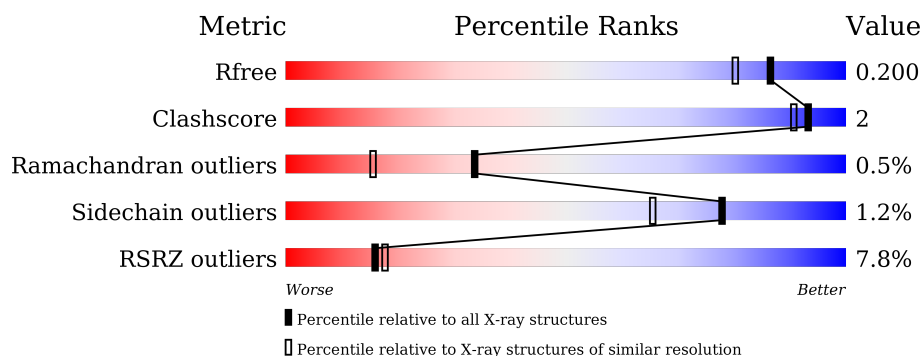
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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  $\geq 3$ , 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>92%</div> <div>5%</div> <div>.</div> </div>
1	B	483	<div> <div>11%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	C	483	<div> <div>7%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	D	483	<div> <div>9%</div> <div>94%</div> <div>.</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	D	1475	-	-	-	X
4	PEG	A	1477	-	-	-	X
4	PEG	B	1477	-	-	-	X
4	PEG	C	1475	-	-	-	X
5	PGE	A	1479	-	-	-	X
5	PGE	B	1476	-	-	-	X
5	PGE	D	1476	-	-	-	X
6	PG4	C	1478	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16190 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 TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	1	0
			3695	2344	624	707	20			
1	B	473	Total	C	N	O	S	0	1	0
			3733	2367	630	717	19			
1	C	468	Total	C	N	O	S	0	0	0
			3687	2339	623	706	19			
1	D	473	Total	C	N	O	S	0	1	0
			3732	2367	630	715	20			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLN	PRO	CONFLICT	UNP A0A0Q9UXH
A	90	ALA	SER	CONFLICT	UNP A0A0Q9UXH
A	202	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
A	205	LEU	CYS	CONFLICT	UNP A0A0Q9UXH
A	268	ASN	THR	CONFLICT	UNP A0A0Q9UXH
A	318	ALA	GLU	CONFLICT	UNP A0A0Q9UXH
A	322	LYS	ARG	CONFLICT	UNP A0A0Q9UXH
A	359	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
A	452	GLY	GLU	CONFLICT	UNP A0A0Q9UXH
A	475	ALA	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	476	LEU	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	477	GLU	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	478	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	479	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	480	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	481	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	482	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
A	483	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	69	GLN	PRO	CONFLICT	UNP A0A0Q9UXH
B	90	ALA	SER	CONFLICT	UNP A0A0Q9UXH
B	202	ASP	ASN	CONFLICT	UNP A0A0Q9UXH

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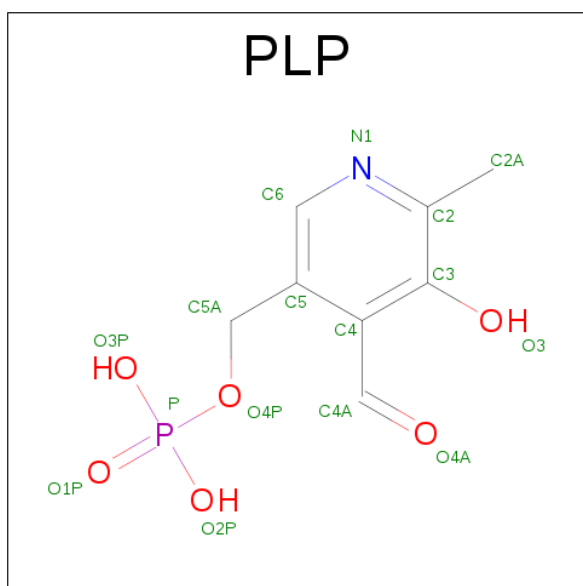
Chain	Residue	Modelled	Actual	Comment	Reference
B	205	LEU	CYS	CONFLICT	UNP A0A0Q9UXH
B	268	ASN	THR	CONFLICT	UNP A0A0Q9UXH
B	318	ALA	GLU	CONFLICT	UNP A0A0Q9UXH
B	322	LYS	ARG	CONFLICT	UNP A0A0Q9UXH
B	359	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
B	452	GLY	GLU	CONFLICT	UNP A0A0Q9UXH
B	475	ALA	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	476	LEU	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	477	GLU	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	478	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	479	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	480	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	481	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	482	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
B	483	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	69	GLN	PRO	CONFLICT	UNP A0A0Q9UXH
C	90	ALA	SER	CONFLICT	UNP A0A0Q9UXH
C	202	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
C	205	LEU	CYS	CONFLICT	UNP A0A0Q9UXH
C	268	ASN	THR	CONFLICT	UNP A0A0Q9UXH
C	318	ALA	GLU	CONFLICT	UNP A0A0Q9UXH
C	322	LYS	ARG	CONFLICT	UNP A0A0Q9UXH
C	359	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
C	452	GLY	GLU	CONFLICT	UNP A0A0Q9UXH
C	475	ALA	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	476	LEU	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	477	GLU	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	478	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	479	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	480	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	481	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	482	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
C	483	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	69	GLN	PRO	CONFLICT	UNP A0A0Q9UXH
D	90	ALA	SER	CONFLICT	UNP A0A0Q9UXH
D	202	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
D	205	LEU	CYS	CONFLICT	UNP A0A0Q9UXH
D	268	ASN	THR	CONFLICT	UNP A0A0Q9UXH
D	318	ALA	GLU	CONFLICT	UNP A0A0Q9UXH
D	322	LYS	ARG	CONFLICT	UNP A0A0Q9UXH
D	359	ASP	ASN	CONFLICT	UNP A0A0Q9UXH
D	452	GLY	GLU	CONFLICT	UNP A0A0Q9UXH

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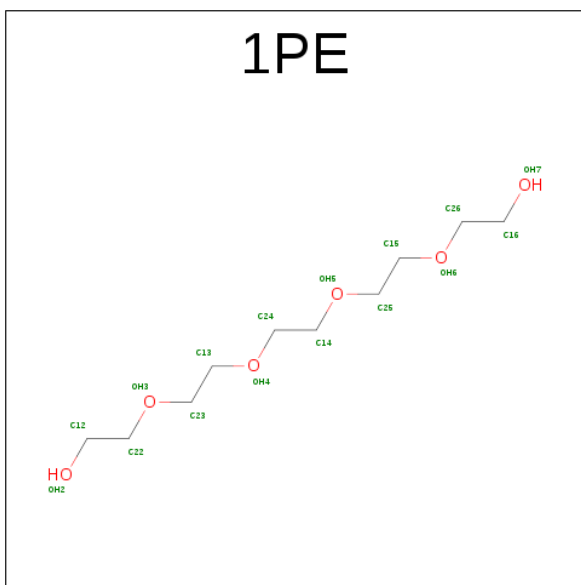
Chain	Residue	Modelled	Actual	Comment	Reference
D	475	ALA	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	476	LEU	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	477	GLU	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	478	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	479	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	480	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	481	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	482	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH
D	483	HIS	-	EXPRESSION TAG	UNP A0A0Q9UXH

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



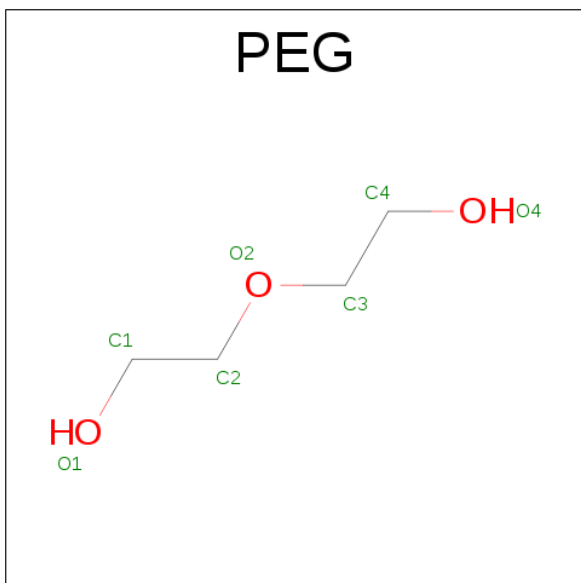
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



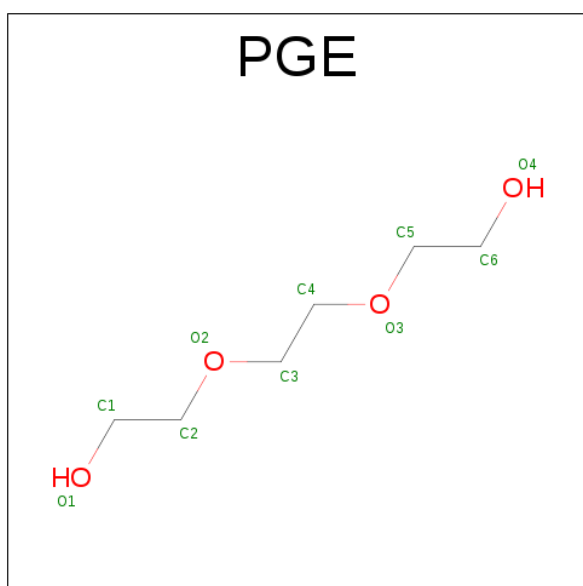
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

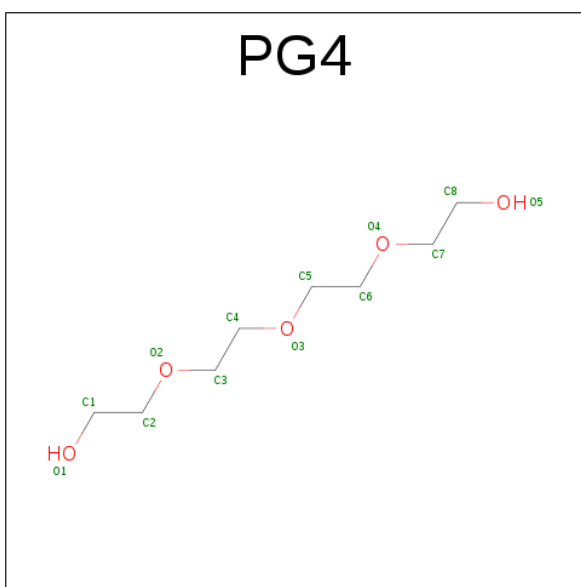
- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		

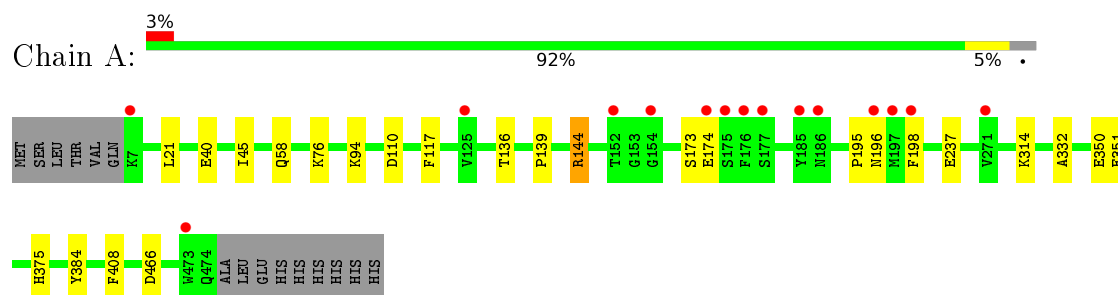
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	371	Total	O	0	0
			371	371		
7	B	236	Total	O	0	0
			236	236		
7	C	285	Total	O	0	0
			285	285		
7	D	204	Total	O	0	0
			204	204		

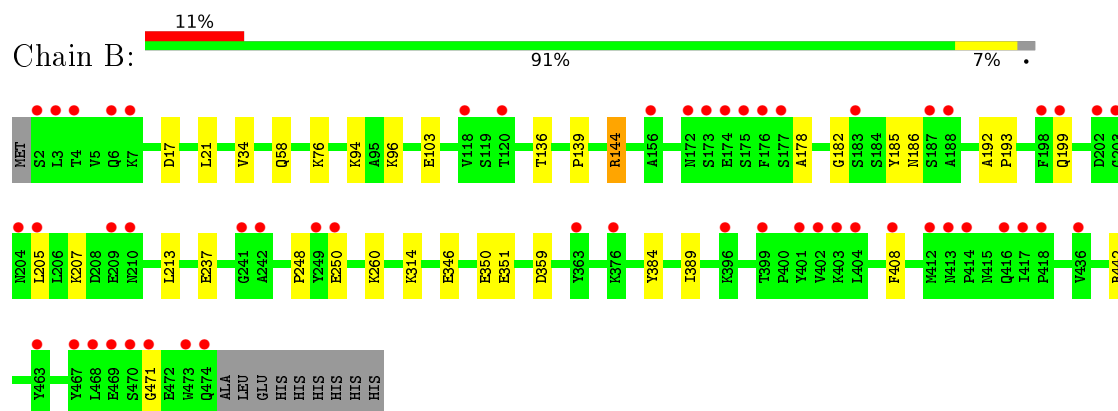
### 3 Residue-property plots [i](#)

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.

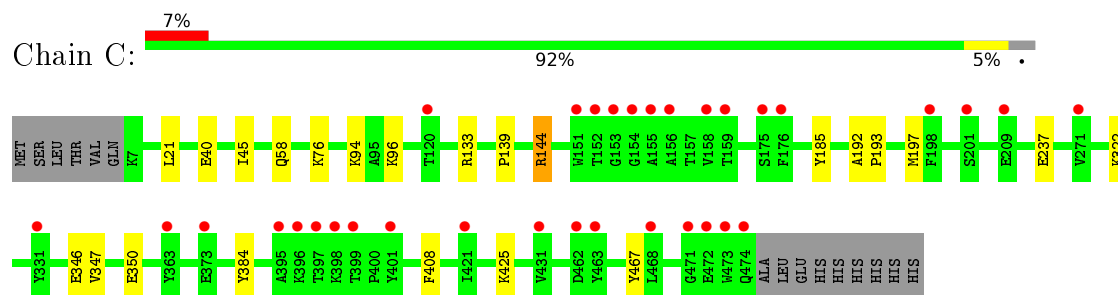
#### • Molecule 1: TRANSAMINASE



#### • Molecule 1: TRANSAMINASE

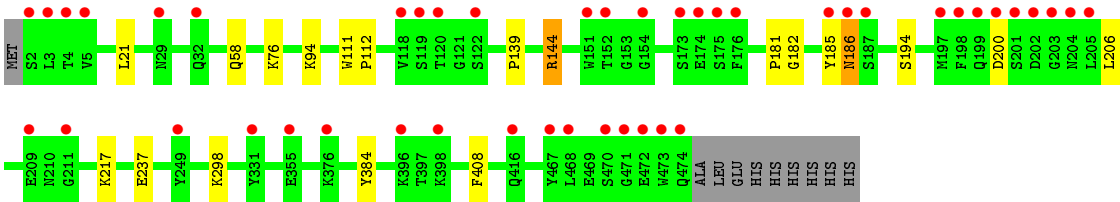


#### • Molecule 1: TRANSAMINASE



#### • Molecule 1: TRANSAMINASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.14Å 124.64Å 126.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.42 – 1.70 43.42 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.42-1.70) 96.6 (43.42-1.70)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.172 , 0.200 0.173 , 0.200	Depositor DCC
$R_{free}$ test set	9934 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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: PEG, PG4, PGE, 1PE, 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	0.54	0/3776	0.65	0/5114
1	B	0.50	0/3814	0.65	0/5167
1	C	0.47	0/3768	0.63	0/5104
1	D	0.49	0/3813	0.63	0/5165
All	All	0.50	0/15171	0.64	0/20550

There are no bond length outliers.

There are no bond angle outliers.

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	3695	0	3630	13	0
1	B	3733	0	3667	23	0
1	C	3687	0	3622	14	0
1	D	3732	0	3670	12	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
3	A	48	0	66	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	16	0	22	2	0
4	A	7	0	10	0	0
4	B	14	0	20	2	0
4	C	7	0	10	0	0
5	A	10	0	14	2	0
5	B	10	0	14	4	0
5	D	10	0	14	0	0
6	B	13	0	18	1	0
6	C	52	0	72	0	0
7	A	371	0	0	3	0
7	B	236	0	0	3	0
7	C	285	0	0	3	0
7	D	204	0	0	0	0
All	All	16190	0	14873	58	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 2.

All (58) 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:40:GLU:HG2	1:A:45:ILE:HD11	1.67	0.74
1:C:21:LEU:HD13	1:D:94:LYS:HE3	1.72	0.70
1:B:96:LYS:CE	1:B:346:GLU:OE2	2.41	0.68
1:B:182:GLY:HA2	1:B:185:TYR:CE1	2.33	0.63
1:D:182:GLY:HA2	1:D:185:TYR:CD1	2.35	0.61
1:C:94:LYS:HE3	1:D:21:LEU:HD13	1.82	0.60
1:A:21:LEU:HD13	1:B:94:LYS:HE3	1.83	0.59
5:B:1476:PGE:H1	7:B:2106:HOH:O	2.01	0.59
1:B:34:VAL:HG21	6:B:1478:PG4:H81	1.85	0.58
7:A:2150:HOH:O	1:B:178:ALA:HB1	2.04	0.57
1:B:182:GLY:HA2	1:B:185:TYR:CD1	2.39	0.57
1:C:40:GLU:HG2	1:C:45:ILE:HD11	1.86	0.57
1:A:76:LYS:HG2	1:B:76:LYS:HG2	1.87	0.55
1:A:94:LYS:HE3	1:B:21:LEU:HD13	1.89	0.55
5:B:1476:PGE:H52	7:B:2106:HOH:O	2.08	0.54
1:A:136:THR:HG22	5:A:1479:PGE:H42	1.91	0.53
1:B:260:LYS:HZ1	4:B:1477:PEG:H22	1.73	0.53
1:C:322:LYS:HE2	7:C:2235:HOH:O	2.10	0.52
1:C:185:TYR:O	1:D:186:ASN:OD1	2.28	0.52
1:B:96:LYS:NZ	1:B:346:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:CD1	1:D:94:LYS:HE3	2.41	0.51
1:B:199:GLN:HG2	1:B:205:LEU:HD13	1.94	0.50
1:B:260:LYS:NZ	4:B:1477:PEG:H22	2.27	0.50
1:B:17:ASP:HA	1:B:21:LEU:HD12	1.94	0.50
1:B:103[A]:GLU:OE1	1:B:103[A]:GLU:HA	2.13	0.49
1:D:182:GLY:HA2	1:D:185:TYR:CE1	2.48	0.49
1:D:200:ASP:HB3	1:D:206:LEU:HD21	1.93	0.49
7:C:2085:HOH:O	3:D:1475:1PE:H241	2.13	0.49
1:B:350:GLU:HG2	1:B:351:GLU:HG3	1.93	0.48
1:B:389:ILE:HG23	1:B:442:ARG:NH1	2.30	0.47
1:A:198:PHE:CE1	1:D:217:LYS:HD3	2.50	0.46
5:A:1479:PGE:H6	7:A:2146:HOH:O	2.16	0.46
1:C:76:LYS:HG2	1:D:76:LYS:HG2	1.98	0.45
1:C:425:LYS:HG3	1:C:467:TYR:CD2	2.52	0.45
1:B:136:THR:HG22	5:B:1476:PGE:H3	1.98	0.45
7:C:2249:HOH:O	3:D:1475:1PE:H162	2.17	0.45
1:C:192:ALA:HB1	1:C:193:PRO:HD2	1.99	0.44
1:B:314:LYS:NZ	7:B:2089:HOH:O	2.35	0.44
1:A:173:SER:OG	1:A:174:GLU:N	2.51	0.43
1:C:347:VAL:HA	1:C:350:GLU:HG2	2.01	0.43
1:D:144:ARG:NH2	1:D:237:GLU:H	2.16	0.43
1:D:111:TRP:CD1	1:D:112:PRO:HD3	2.54	0.43
1:B:144:ARG:NH2	1:B:237:GLU:H	2.17	0.42
1:B:205:LEU:HG	1:B:248:PRO:HG3	2.01	0.42
1:C:144:ARG:NH2	1:C:237:GLU:H	2.17	0.42
1:C:96:LYS:HE2	1:C:346:GLU:OE2	2.18	0.42
1:A:195:PRO:O	1:A:196:ASN:HB2	2.18	0.42
1:C:425:LYS:HE3	1:C:467:TYR:CD1	2.55	0.42
1:B:192:ALA:HB1	1:B:193:PRO:HD2	2.01	0.42
1:A:314:LYS:NZ	7:A:2120:HOH:O	2.41	0.42
5:B:1476:PGE:H32	5:B:1476:PGE:H1	1.86	0.42
1:B:96:LYS:HE3	1:B:346:GLU:OE2	2.16	0.42
1:C:133:ARG:HB3	1:D:181:PRO:HD2	2.03	0.41
1:A:375:HIS:HE1	1:A:466:ASP:OD1	2.04	0.41
1:B:207:LYS:HG2	1:B:213:LEU:HD23	2.03	0.41
1:A:350:GLU:HG3	1:A:351:GLU:HG3	2.03	0.41
1:A:117:PHE:O	1:A:332:ALA:HB1	2.21	0.40
1:A:144:ARG:NH2	1:A:237:GLU:H	2.19	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	467/483 (97%)	453 (97%)	12 (3%)	2 (0%)	39	20
1	B	472/483 (98%)	451 (96%)	18 (4%)	3 (1%)	30	12
1	C	466/483 (96%)	451 (97%)	13 (3%)	2 (0%)	39	20
1	D	472/483 (98%)	454 (96%)	15 (3%)	3 (1%)	30	12
All	All	1877/1932 (97%)	1809 (96%)	58 (3%)	10 (0%)	34	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	GLY
1	A	58	GLN
1	B	58	GLN
1	C	58	GLN
1	D	58	GLN
1	D	298	LYS
1	B	139	PRO
1	D	139	PRO
1	C	139	PRO
1	A	139	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	395/408 (97%)	391 (99%)	4 (1%)	82	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	400/408 (98%)	394 (98%)	6 (2%)	72	56
1	C	394/408 (97%)	390 (99%)	4 (1%)	82	72
1	D	400/408 (98%)	395 (99%)	5 (1%)	76	62
All	All	1589/1632 (97%)	1570 (99%)	19 (1%)	78	65

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

Mol	Chain	Res	Type
1	A	110	ASP
1	A	144	ARG
1	A	384	TYR
1	A	408	PHE
1	B	144	ARG
1	B	186	ASN
1	B	250	GLU
1	B	359	ASP
1	B	384	TYR
1	B	408	PHE
1	C	144	ARG
1	C	197	MET
1	C	384	TYR
1	C	408	PHE
1	D	144	ARG
1	D	186	ASN
1	D	194	SER
1	D	384	TYR
1	D	408	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	268	ASN
1	B	268	ASN
1	C	268	ASN
1	D	268	ASN

### 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 ⓘ

20 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	A	1298	1	15,15,16	2.84	3 (20%)	21,22,23	1.36	3 (14%)
3	1PE	A	1475	-	15,15,15	0.55	0	14,14,14	0.33	0
3	1PE	A	1476	-	15,15,15	0.47	0	14,14,14	0.35	0
4	PEG	A	1477	-	6,6,6	0.48	0	5,5,5	0.19	0
3	1PE	A	1478	-	15,15,15	0.49	0	14,14,14	0.34	0
5	PGE	A	1479	-	9,9,9	0.49	0	8,8,8	0.60	0
2	PLP	B	1298	1	15,15,16	3.56	3 (20%)	21,22,23	1.65	5 (23%)
4	PEG	B	1475	-	6,6,6	0.43	0	5,5,5	0.38	0
5	PGE	B	1476	-	9,9,9	0.47	0	8,8,8	0.45	0
4	PEG	B	1477	-	6,6,6	0.56	0	5,5,5	0.40	0
6	PG4	B	1478	-	12,12,12	0.41	0	11,11,11	0.40	0
2	PLP	C	1298	1	15,15,16	3.26	3 (20%)	21,22,23	1.55	3 (14%)
4	PEG	C	1475	-	6,6,6	0.50	0	5,5,5	0.32	0
6	PG4	C	1476	-	12,12,12	0.44	0	11,11,11	0.42	0
6	PG4	C	1477	-	12,12,12	0.53	0	11,11,11	0.41	0
6	PG4	C	1478	-	12,12,12	0.43	0	11,11,11	0.50	0
6	PG4	C	1479	-	12,12,12	0.49	0	11,11,11	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	D	1298	1	15,15,16	3.26	3 (20%)	21,22,23	1.49	5 (23%)
3	1PE	D	1475	-	15,15,15	0.49	0	14,14,14	0.36	0
5	PGE	D	1476	-	9,9,9	0.44	0	8,8,8	0.33	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	A	1298	1	-	0/6/6/8	0/1/1/1
3	1PE	A	1475	-	-	0/13/13/13	0/0/0/0
3	1PE	A	1476	-	-	0/13/13/13	0/0/0/0
4	PEG	A	1477	-	-	0/4/4/4	0/0/0/0
3	1PE	A	1478	-	-	0/13/13/13	0/0/0/0
5	PGE	A	1479	-	-	0/7/7/7	0/0/0/0
2	PLP	B	1298	1	-	0/6/6/8	0/1/1/1
4	PEG	B	1475	-	-	0/4/4/4	0/0/0/0
5	PGE	B	1476	-	-	0/7/7/7	0/0/0/0
4	PEG	B	1477	-	-	0/4/4/4	0/0/0/0
6	PG4	B	1478	-	-	0/10/10/10	0/0/0/0
2	PLP	C	1298	1	-	0/6/6/8	0/1/1/1
4	PEG	C	1475	-	-	0/4/4/4	0/0/0/0
6	PG4	C	1476	-	-	0/10/10/10	0/0/0/0
6	PG4	C	1477	-	-	0/10/10/10	0/0/0/0
6	PG4	C	1478	-	-	0/10/10/10	0/0/0/0
6	PG4	C	1479	-	-	0/10/10/10	0/0/0/0
2	PLP	D	1298	1	-	0/6/6/8	0/1/1/1
3	1PE	D	1475	-	-	0/13/13/13	0/0/0/0
5	PGE	D	1476	-	-	0/7/7/7	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1298	PLP	C3-C4	3.30	1.47	1.40
2	D	1298	PLP	C3-C4	3.39	1.47	1.40
2	C	1298	PLP	C3-C4	3.43	1.47	1.40
2	A	1298	PLP	C3-C4	3.57	1.48	1.40
2	A	1298	PLP	C5-C4	6.09	1.47	1.40
2	D	1298	PLP	C5-C4	6.88	1.48	1.40
2	B	1298	PLP	C5-C4	6.96	1.48	1.40
2	C	1298	PLP	C5-C4	7.83	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1298	PLP	C3-C2	7.96	1.46	1.40
2	C	1298	PLP	C3-C2	8.93	1.47	1.40
2	D	1298	PLP	C3-C2	9.68	1.47	1.40
2	B	1298	PLP	C3-C2	11.10	1.48	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1298	PLP	O4P-P-O1P	-2.85	99.92	107.08
2	B	1298	PLP	C3-C4-C5	-2.61	115.63	118.68
2	D	1298	PLP	C2A-C2-C3	-2.37	118.50	120.90
2	C	1298	PLP	O4P-P-O1P	-2.25	101.42	107.08
2	D	1298	PLP	O4P-P-O1P	-2.12	101.76	107.08
2	A	1298	PLP	C2A-C2-C3	-2.03	118.84	120.90
2	A	1298	PLP	C4A-C4-C5	2.10	123.06	120.90
2	D	1298	PLP	C2A-C2-N1	2.15	122.71	117.96
2	D	1298	PLP	C6-N1-C2	2.30	123.88	119.26
2	C	1298	PLP	C4A-C4-C5	2.36	123.32	120.90
2	A	1298	PLP	C6-N1-C2	2.48	124.24	119.26
2	D	1298	PLP	C4A-C4-C5	2.65	123.63	120.90
2	B	1298	PLP	C6-C5-C4	2.77	120.48	118.12
2	C	1298	PLP	C6-N1-C2	3.06	125.41	119.26
2	B	1298	PLP	C4A-C4-C5	3.15	124.14	120.90
2	B	1298	PLP	O3-C3-C2	3.15	122.15	117.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1479	PGE	2	0
5	B	1476	PGE	4	0
4	B	1477	PEG	2	0
6	B	1478	PG4	1	0
3	D	1475	1PE	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	468/483 (96%)	0.12	15 (3%) 51 55	20, 28, 41, 57	0
1	B	473/483 (97%)	0.66	53 (11%) 7 8	20, 30, 57, 83	0
1	C	468/483 (96%)	0.43	33 (7%) 19 21	22, 32, 51, 78	0
1	D	473/483 (97%)	0.47	45 (9%) 10 11	22, 31, 53, 71	0
All	All	1882/1932 (97%)	0.42	146 (7%) 16 18	20, 30, 52, 83	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	PHE	14.2
1	D	3	LEU	10.3
1	D	201	SER	8.7
1	B	471	GLY	8.2
1	B	3	LEU	7.5
1	D	176	PHE	7.4
1	D	4	THR	7.2
1	B	175	SER	7.0
1	D	473	TRP	6.7
1	C	471	GLY	6.3
1	A	176	PHE	6.3
1	B	174	GLU	6.3
1	C	176	PHE	6.1
1	A	198	PHE	5.7
1	B	474	GLN	5.4
1	B	473	TRP	5.4
1	D	205	LEU	5.4
1	C	396	LYS	5.2
1	D	202	ASP	5.2
1	A	175	SER	5.1
1	C	198	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	203	GLY	5.1
1	B	210	ASN	4.9
1	D	198	PHE	4.9
1	D	471	GLY	4.9
1	C	473	TRP	4.6
1	C	175	SER	4.5
1	B	2	SER	4.4
1	B	468	LEU	4.4
1	B	209	GLU	4.3
1	B	6	GLN	4.2
1	B	7	LYS	4.0
1	D	204	ASN	4.0
1	D	5	VAL	4.0
1	B	412	MET	3.9
1	D	249	TYR	3.9
1	B	414	PRO	3.8
1	D	416	GLN	3.6
1	B	4	THR	3.6
1	B	417	ILE	3.6
1	C	151	TRP	3.4
1	B	183	SER	3.4
1	D	32	GLN	3.4
1	B	416	GLN	3.3
1	B	401	TYR	3.3
1	D	200	ASP	3.3
1	C	397	THR	3.3
1	B	203	GLY	3.2
1	B	177	SER	3.2
1	C	395	ALA	3.2
1	D	474	GLN	3.2
1	D	187	SER	3.2
1	B	418	PRO	3.1
1	B	402	VAL	3.1
1	D	199	GLN	3.0
1	B	413	ASN	3.0
1	B	242	ALA	2.9
1	C	156	ALA	2.9
1	B	202	ASP	2.9
1	D	118	VAL	2.9
1	A	197	MET	2.9
1	C	398	LYS	2.9
1	B	470	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	2	SER	2.8
1	D	186	ASN	2.8
1	B	403	LYS	2.8
1	B	173	SER	2.8
1	B	172	ASN	2.8
1	C	271	VAL	2.8
1	B	467	TYR	2.7
1	D	209	GLU	2.7
1	B	250	GLU	2.7
1	D	173	SER	2.7
1	C	472	GLU	2.7
1	D	396	LYS	2.7
1	B	204	ASN	2.7
1	A	7	LYS	2.7
1	D	152	THR	2.7
1	D	175	SER	2.7
1	B	376	LYS	2.6
1	A	196	ASN	2.6
1	B	187	SER	2.6
1	C	463	TYR	2.6
1	C	399	THR	2.6
1	D	185	TYR	2.6
1	B	205	LEU	2.5
1	B	399	THR	2.5
1	B	118	VAL	2.5
1	C	331	TYR	2.5
1	C	153	GLY	2.5
1	D	29	ASN	2.4
1	D	174	GLU	2.4
1	C	120	THR	2.4
1	D	398	LYS	2.4
1	B	241	GLY	2.4
1	C	158	VAL	2.4
1	D	197	MET	2.4
1	C	201	SER	2.4
1	D	376	LYS	2.4
1	C	468	LEU	2.4
1	C	363	TYR	2.3
1	C	401	TYR	2.3
1	D	472	GLU	2.3
1	B	120	THR	2.3
1	B	396	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	404	LEU	2.3
1	C	159	THR	2.3
1	D	151	TRP	2.3
1	B	249	TYR	2.3
1	B	463	TYR	2.3
1	C	431	VAL	2.3
1	A	186	ASN	2.3
1	D	468	LEU	2.3
1	B	469	GLU	2.3
1	C	209	GLU	2.3
1	D	154	GLY	2.3
1	A	473	TRP	2.2
1	D	120	THR	2.2
1	A	185	TYR	2.2
1	D	331	TYR	2.2
1	C	152	THR	2.2
1	B	156	ALA	2.2
1	B	436	VAL	2.2
1	C	154	GLY	2.2
1	C	155	ALA	2.2
1	B	198	PHE	2.2
1	C	421	ILE	2.2
1	B	408	PHE	2.1
1	C	373	GLU	2.1
1	D	355	GLU	2.1
1	A	152	THR	2.1
1	C	462	ASP	2.1
1	A	154	GLY	2.1
1	B	199	GLN	2.1
1	C	474	GLN	2.1
1	B	363	TYR	2.1
1	D	119	SER	2.1
1	D	122	SER	2.1
1	D	470	SER	2.1
1	D	467	TYR	2.1
1	A	125	VAL	2.1
1	D	211	GLY	2.1
1	B	188	ALA	2.0
1	A	271	VAL	2.0
1	A	177	SER	2.0
1	A	174	GLU	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
4	PEG	A	1477	7/7	0.80	0.26	6.14	51,53,57,62	0
6	PG4	C	1478	13/13	0.89	0.21	5.94	38,41,47,51	0
5	PGE	B	1476	10/10	0.86	0.16	5.37	33,38,43,45	0
4	PEG	C	1475	7/7	0.82	0.22	4.94	47,49,52,56	0
4	PEG	B	1477	7/7	0.80	0.15	4.01	43,45,49,50	0
5	PGE	D	1476	10/10	0.87	0.22	3.35	43,47,49,53	0
3	1PE	D	1475	16/16	0.82	0.17	3.21	44,50,57,60	0
5	PGE	A	1479	10/10	0.83	0.15	2.67	40,45,50,51	0
4	PEG	B	1475	7/7	0.79	0.12	1.75	56,58,59,60	0
3	1PE	A	1475	16/16	0.87	0.14	1.13	35,38,52,54	0
6	PG4	C	1477	13/13	0.87	0.15	1.13	40,43,51,52	0
6	PG4	B	1478	13/13	0.87	0.13	0.72	45,51,68,71	0
3	1PE	A	1478	16/16	0.76	0.19	0.19	49,53,56,56	0
2	PLP	A	1298	15/16	0.97	0.14	0.16	20,23,27,28	0
2	PLP	C	1298	15/16	0.97	0.15	-0.07	23,25,28,31	0
6	PG4	C	1476	13/13	0.83	0.15	-0.36	52,54,57,61	0
2	PLP	B	1298	15/16	0.97	0.12	-0.69	22,23,27,30	0
2	PLP	D	1298	15/16	0.97	0.13	-0.80	24,25,28,31	0
6	PG4	C	1479	13/13	0.83	0.23	-	50,56,58,60	0
3	1PE	A	1476	16/16	0.88	0.20	-	40,49,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.