



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 12:56 PM EDT

PDB ID : 3LXM  
Title : 2.00 Angstrom resolution crystal structure of a catalytic subunit of an aspartate carbamoyltransferase (pyrB) from *Yersinia pestis* CO92  
Authors : Halavaty, A.S.; Minasov, G.; Dubrovskaya, I.; Winsor, J.; Shuvalova, L.; Peterson, S.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2010-02-25  
Resolution : 2.00 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

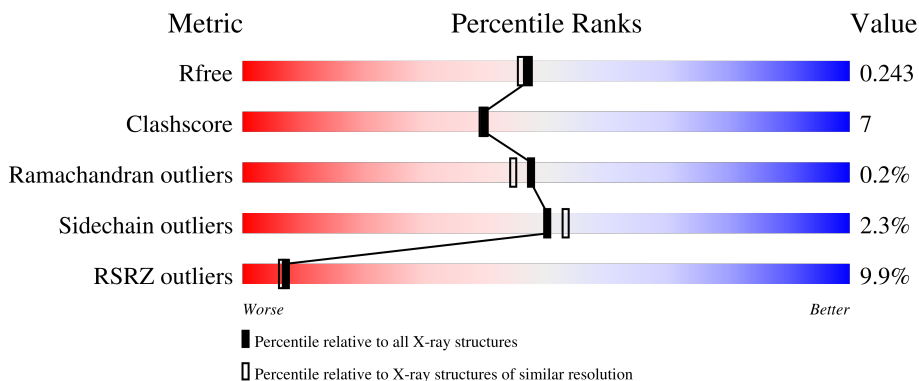
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	335	 5% 76% 9% • 13%
1	B	335	 11% 68% 15% • 16%
1	C	335	 10% 69% 13% • 17%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7196 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	Total 2316	C 1471	N 395	O 442	S 8	0	5	0
1	B	282	Total 2244	C 1427	N 385	O 425	S 7	0	3	0
1	C	277	Total 2171	C 1379	N 368	O 416	S 8	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q8ZB39
A	-22	HIS	-	expression tag	UNP Q8ZB39
A	-21	HIS	-	expression tag	UNP Q8ZB39
A	-20	HIS	-	expression tag	UNP Q8ZB39
A	-19	HIS	-	expression tag	UNP Q8ZB39
A	-18	HIS	-	expression tag	UNP Q8ZB39
A	-17	HIS	-	expression tag	UNP Q8ZB39
A	-16	SER	-	expression tag	UNP Q8ZB39
A	-15	SER	-	expression tag	UNP Q8ZB39
A	-14	GLY	-	expression tag	UNP Q8ZB39
A	-13	VAL	-	expression tag	UNP Q8ZB39
A	-12	ASP	-	expression tag	UNP Q8ZB39
A	-11	LEU	-	expression tag	UNP Q8ZB39
A	-10	GLY	-	expression tag	UNP Q8ZB39
A	-9	THR	-	expression tag	UNP Q8ZB39
A	-8	GLU	-	expression tag	UNP Q8ZB39
A	-7	ASN	-	expression tag	UNP Q8ZB39
A	-6	LEU	-	expression tag	UNP Q8ZB39
A	-5	TYR	-	expression tag	UNP Q8ZB39
A	-4	PHE	-	expression tag	UNP Q8ZB39
A	-3	GLN	-	expression tag	UNP Q8ZB39
A	-2	SER	-	expression tag	UNP Q8ZB39
A	-1	ASN	-	expression tag	UNP Q8ZB39

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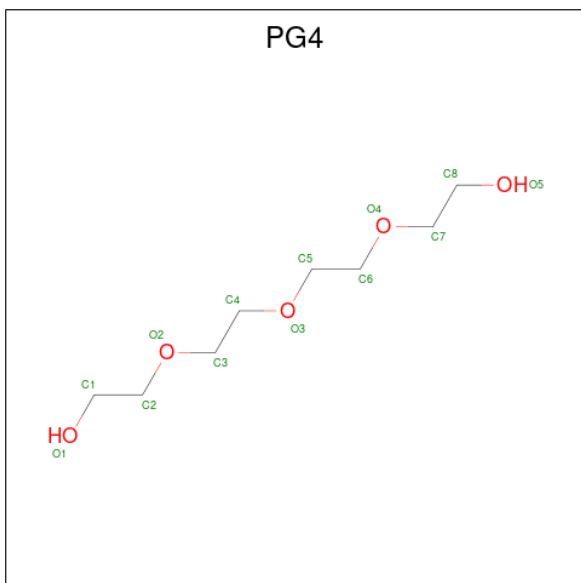
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q8ZB39
B	-23	MET	-	expression tag	UNP Q8ZB39
B	-22	HIS	-	expression tag	UNP Q8ZB39
B	-21	HIS	-	expression tag	UNP Q8ZB39
B	-20	HIS	-	expression tag	UNP Q8ZB39
B	-19	HIS	-	expression tag	UNP Q8ZB39
B	-18	HIS	-	expression tag	UNP Q8ZB39
B	-17	HIS	-	expression tag	UNP Q8ZB39
B	-16	SER	-	expression tag	UNP Q8ZB39
B	-15	SER	-	expression tag	UNP Q8ZB39
B	-14	GLY	-	expression tag	UNP Q8ZB39
B	-13	VAL	-	expression tag	UNP Q8ZB39
B	-12	ASP	-	expression tag	UNP Q8ZB39
B	-11	LEU	-	expression tag	UNP Q8ZB39
B	-10	GLY	-	expression tag	UNP Q8ZB39
B	-9	THR	-	expression tag	UNP Q8ZB39
B	-8	GLU	-	expression tag	UNP Q8ZB39
B	-7	ASN	-	expression tag	UNP Q8ZB39
B	-6	LEU	-	expression tag	UNP Q8ZB39
B	-5	TYR	-	expression tag	UNP Q8ZB39
B	-4	PHE	-	expression tag	UNP Q8ZB39
B	-3	GLN	-	expression tag	UNP Q8ZB39
B	-2	SER	-	expression tag	UNP Q8ZB39
B	-1	ASN	-	expression tag	UNP Q8ZB39
B	0	ALA	-	expression tag	UNP Q8ZB39
C	-23	MET	-	expression tag	UNP Q8ZB39
C	-22	HIS	-	expression tag	UNP Q8ZB39
C	-21	HIS	-	expression tag	UNP Q8ZB39
C	-20	HIS	-	expression tag	UNP Q8ZB39
C	-19	HIS	-	expression tag	UNP Q8ZB39
C	-18	HIS	-	expression tag	UNP Q8ZB39
C	-17	HIS	-	expression tag	UNP Q8ZB39
C	-16	SER	-	expression tag	UNP Q8ZB39
C	-15	SER	-	expression tag	UNP Q8ZB39
C	-14	GLY	-	expression tag	UNP Q8ZB39
C	-13	VAL	-	expression tag	UNP Q8ZB39
C	-12	ASP	-	expression tag	UNP Q8ZB39
C	-11	LEU	-	expression tag	UNP Q8ZB39
C	-10	GLY	-	expression tag	UNP Q8ZB39
C	-9	THR	-	expression tag	UNP Q8ZB39
C	-8	GLU	-	expression tag	UNP Q8ZB39
C	-7	ASN	-	expression tag	UNP Q8ZB39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	expression tag	UNP Q8ZB39
C	-5	TYR	-	expression tag	UNP Q8ZB39
C	-4	PHE	-	expression tag	UNP Q8ZB39
C	-3	GLN	-	expression tag	UNP Q8ZB39
C	-2	SER	-	expression tag	UNP Q8ZB39
C	-1	ASN	-	expression tag	UNP Q8ZB39
C	0	ALA	-	expression tag	UNP Q8ZB39

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).

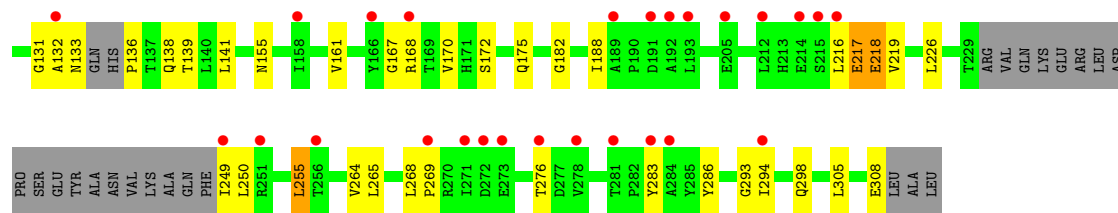


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	230	Total O 234 234	0	4
3	B	106	Total O 106 106	0	0
3	C	112	Total O 112 112	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.62Å 120.41Å 126.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.83 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.00) 99.6 (29.83-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.179 , 0.217 0.210 , 0.243	Depositor DCC
$R_{free}$ test set	3574 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: PG4

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	0.84	0/2359	0.93	7/3200 (0.2%)
1	B	0.66	0/2287	0.81	4/3104 (0.1%)
1	C	0.64	0/2209	0.79	4/2994 (0.1%)
All	All	0.72	0/6855	0.85	15/9298 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	GLU	CB-CA-C	-9.73	90.93	110.40
1	A	141	LEU	CA-CB-CG	7.80	133.24	115.30
1	C	93	MET	CG-SD-CE	-7.61	88.02	100.20
1	A	114	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	114	ARG	CB-CA-C	-6.24	97.92	110.40
1	B	99[A]	TYR	CB-CA-C	-6.09	98.22	110.40
1	B	99[B]	TYR	CB-CA-C	-6.09	98.22	110.40
1	A	114	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	141	LEU	CB-CG-CD2	5.35	120.09	111.00
1	B	99[A]	TYR	CA-CB-CG	5.29	123.45	113.40
1	B	99[B]	TYR	CA-CB-CG	5.29	123.45	113.40
1	A	55	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	C	18	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	18	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	219	VAL	N-CA-CB	5.12	122.77	111.50

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	2316	0	2298	24	0
1	B	2244	0	2235	41	0
1	C	2171	0	2169	33	0
2	A	13	0	18	2	0
3	A	234	0	0	2	0
3	B	106	0	0	8	0
3	C	112	0	0	4	0
All	All	7196	0	6720	98	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 7.

All (98) 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:89:LEU:HD21	1:A:105[B]:MET:CE	1.70	1.21
1:A:89:LEU:CD2	1:A:105[B]:MET:HE1	1.75	1.14
1:B:247:GLN:HE21	1:B:247:GLN:HA	1.03	1.12
1:B:247:GLN:HA	1:B:247:GLN:NE2	1.78	0.97
1:B:247:GLN:HE21	1:B:247:GLN:CA	1.83	0.87
1:A:271:ILE:HG12	3:C:391:HOH:O	1.74	0.86
1:C:255:LEU:HD12	1:C:283:TYR:CD2	2.18	0.79
1:B:21:LEU:CD1	3:B:353:HOH:O	2.31	0.77
1:B:168:ARG:HG2	1:B:169:THR:H	1.51	0.74
1:A:53:SER:OG	2:A:312:PG4:H41	1.88	0.73
1:B:273:GLU:OE2	1:B:273:GLU:N	2.20	0.72
1:A:99[A]:TYR:CE1	3:B:331:HOH:O	2.45	0.69
1:B:33:LYS:HG2	1:B:34:THR:HG23	1.75	0.69
1:A:89:LEU:HD21	1:A:105[B]:MET:HE1	0.79	0.66
1:C:141:LEU:HD22	1:C:293:GLY:HA2	1.78	0.66
1:C:216:LEU:HD11	1:C:226:LEU:HD21	1.79	0.63
1:B:168:ARG:H	1:B:168:ARG:HD2	1.63	0.63
1:A:230:ARG:NH1	1:A:268:LEU:O	2.29	0.62
1:B:167:GLY:O	1:B:170:VAL:HG12	2.00	0.61
1:B:218:GLU:HG3	1:B:219:VAL:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:HIS:HD2	1:B:109:GLN:H	1.47	0.61
1:A:308:GLU:H	1:A:308:GLU:CD	2.05	0.60
1:B:196:PRO:O	1:B:200:LEU:HD13	2.02	0.59
1:C:276:THR:CG2	3:C:387:HOH:O	2.51	0.59
1:B:107:HIS:CD2	1:B:108:PRO:HD2	2.38	0.58
1:C:216:LEU:C	1:C:216:LEU:HD23	2.24	0.57
1:B:21:LEU:HD11	3:B:353:HOH:O	1.98	0.56
1:C:139:THR:OG1	1:C:172:SER:OG	2.22	0.55
1:C:76:ASP:OD2	1:C:77:SER:N	2.36	0.55
1:C:249:ILE:O	1:C:249:ILE:HG23	2.07	0.55
1:B:216:LEU:HD21	1:B:226:LEU:HD11	1.90	0.54
1:B:95:VAL:HG13	1:B:96:ILE:N	2.22	0.54
1:C:132:ALA:HB1	1:C:168:ARG:HH11	1.71	0.54
1:C:133:ASN:OD1	1:C:136:PRO:HB3	2.09	0.53
1:C:167:GLY:O	1:C:170:VAL:HG22	2.07	0.53
1:B:76:ASP:OD2	1:B:77:SER:N	2.41	0.53
1:A:137:THR:HG22	1:A:300:LEU:HD12	1.89	0.53
1:B:41:LYS:HE2	3:B:332:HOH:O	2.09	0.53
1:A:99[A]:TYR:HB2	1:A:100:VAL:HG13	1.91	0.52
1:A:245:LYS:O	1:A:249:ILE:HG13	2.10	0.52
1:C:217:GLU:O	1:C:218:GLU:HB2	2.10	0.52
1:C:216:LEU:C	1:C:217:GLU:O	2.42	0.52
1:B:92:THR:O	1:B:95:VAL:HG12	2.10	0.52
1:B:217:GLU:HG3	3:B:391:HOH:O	2.10	0.51
1:C:250:LEU:HD11	1:C:255:LEU:CD2	2.40	0.51
1:A:54:THR:H	2:A:312:PG4:H71	1.76	0.51
1:B:179:LYS:HD3	3:B:353:HOH:O	2.08	0.51
1:C:217:GLU:O	1:C:218:GLU:CB	2.58	0.50
1:C:255:LEU:HD12	1:C:283:TYR:HD2	1.71	0.50
1:A:247:GLN:HG3	1:A:248:PHE:CD1	2.46	0.50
1:A:217:GLU:HB2	3:A:328:HOH:O	2.12	0.49
1:B:39:LEU:HG	1:B:306:ASN:HD21	1.77	0.48
1:C:14:ASN:ND2	3:C:319:HOH:O	2.22	0.48
1:B:127:ASN:HD21	1:B:130:ASP:HB2	1.78	0.48
1:B:33:LYS:HG2	1:B:34:THR:CG2	2.43	0.48
1:B:41:LYS:CE	3:B:332:HOH:O	2.62	0.47
1:C:108:PRO:O	1:C:131:GLY:HA2	2.14	0.47
1:C:308:GLU:HA	1:C:308:GLU:OE1	2.15	0.46
1:C:276:THR:HG23	3:C:387:HOH:O	2.14	0.46
1:C:76:ASP:O	1:C:77:SER:CB	2.63	0.46
1:A:138:GLN:HA	1:A:141:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ALA:HB1	1:C:168:ARG:NH1	2.31	0.46
1:A:105[B]:MET:SD	1:A:115:LEU:HD22	2.57	0.45
1:A:280:LYS:HG2	3:A:506:HOH:O	2.17	0.45
1:B:270:ARG:O	1:B:271:ILE:HD13	2.17	0.45
1:A:37:PRO:HA	1:A:66:ARG:O	2.17	0.45
1:C:155:ASN:HA	1:C:182:GLY:O	2.17	0.44
1:B:147[A]:GLN:OE1	1:B:152:ARG:HA	2.18	0.44
1:C:105[B]:MET:HE1	1:C:116:ALA:CB	2.47	0.44
1:B:16:LEU:HD22	1:B:20:GLU:HB3	1.98	0.44
1:B:67:LEU:HD21	1:B:298:GLN:HE21	1.81	0.44
1:C:161:VAL:HG22	1:C:188:ILE:HB	2.00	0.44
1:B:202:MET:CE	1:B:206:LYS:HD2	2.48	0.44
1:A:249:ILE:HG23	1:A:272:ASP:O	2.18	0.43
1:B:230:ARG:CG	3:B:334:HOH:O	2.66	0.43
1:B:168:ARG:HG2	1:B:169:THR:HG23	1.99	0.43
1:A:137:THR:HG22	1:A:300:LEU:CD1	2.48	0.43
1:A:165:LYS:O	1:A:171:HIS:HE1	2.01	0.43
1:B:141:LEU:C	1:B:141:LEU:HD12	2.39	0.43
1:C:294:ILE:O	1:C:298:GLN:HG3	2.19	0.43
1:B:216:LEU:HD21	1:B:226:LEU:CD1	2.48	0.43
1:A:55:ARG:NH1	1:A:269:PRO:HD3	2.35	0.42
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.89	0.42
1:B:294:ILE:O	1:B:298:GLN:HG3	2.19	0.42
1:A:105[B]:MET:SD	1:A:115:LEU:CD2	3.08	0.42
1:B:37:PRO:HA	1:B:66:ARG:O	2.20	0.42
1:C:138:GLN:HA	1:C:141:LEU:HG	2.02	0.41
1:C:268:LEU:HB3	1:C:269:PRO:HA	2.01	0.41
1:B:39:LEU:HG	1:B:306:ASN:ND2	2.35	0.41
1:B:67:LEU:CD2	1:B:298:GLN:HE21	2.33	0.41
1:B:92:THR:O	1:B:96:ILE:HG12	2.20	0.41
1:C:250:LEU:HD11	1:C:255:LEU:HD22	2.02	0.41
1:C:217:GLU:C	1:C:218:GLU:HG3	2.40	0.41
1:A:89:LEU:CD2	1:A:105[B]:MET:CE	2.60	0.41
1:B:46:ALA:HA	1:B:72:VAL:O	2.21	0.40
1:C:14:ASN:HD21	1:C:175:GLN:HB3	1.87	0.40
1:B:64:ILE:HG21	1:B:71:VAL:HG22	2.04	0.40
1:C:264:VAL:O	1:C:265:LEU:HD12	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	289/335 (86%)	283 (98%)	6 (2%)	0	100	100
1	B	279/335 (83%)	269 (96%)	9 (3%)	1 (0%)	34	30
1	C	270/335 (81%)	259 (96%)	10 (4%)	1 (0%)	34	30
All	All	838/1005 (83%)	811 (97%)	25 (3%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	ARG
1	C	217	GLU

### 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	251/287 (88%)	245 (98%)	6 (2%)	49	51
1	B	245/287 (85%)	238 (97%)	7 (3%)	42	43
1	C	238/287 (83%)	234 (98%)	4 (2%)	60	65
All	All	734/861 (85%)	717 (98%)	17 (2%)	50	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

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Mol	Chain	Res	Type
1	A	141	LEU
1	A	170	VAL
1	A	253	SER
1	A	270	ARG
1	A	308	GLU
1	B	88	THR
1	B	168	ARG
1	B	212	LEU
1	B	247	GLN
1	B	270	ARG
1	B	286	TYR
1	B	308	GLU
1	C	3	ASN
1	C	5	LEU
1	C	255	LEU
1	C	286	TYR

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

Mol	Chain	Res	Type
1	B	107	HIS
1	B	109	GLN
1	B	247	GLN
1	B	306	ASN
1	C	150	GLN
1	C	175	GLN
1	C	181	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 monosaccharides in this entry.

## 5.6 Ligand geometry

1 ligand is 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	PG4	A	312	-	12,12,12	0.71	0	11,11,11	0.47	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	PG4	A	312	-	-	7/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	312	PG4	C3-C4-O3-C5
2	A	312	PG4	O3-C5-C6-O4
2	A	312	PG4	O2-C3-C4-O3
2	A	312	PG4	O1-C1-C2-O2
2	A	312	PG4	C8-C7-O4-C6
2	A	312	PG4	O4-C7-C8-O5
2	A	312	PG4	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	312	PG4	2	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	290/335 (86%)	0.33	16 (5%) 25 24	22, 33, 64, 107	0
1	B	282/335 (84%)	0.59	36 (12%) 3 3	28, 46, 77, 88	0
1	C	277/335 (82%)	0.66	32 (11%) 4 4	25, 51, 100, 116	0
All	All	849/1005 (84%)	0.52	84 (9%) 7 6	22, 44, 82, 116	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	VAL	7.9
1	C	271	ILE	6.4
1	A	241	TYR	6.3
1	A	242	ALA	6.1
1	B	2	ALA	5.9
1	A	243	ASN	5.7
1	A	310	ALA	5.7
1	C	77	SER	5.1
1	C	191	ASP	5.0
1	B	205	GLU	4.8
1	C	214	GLU	4.7
1	C	272	ASP	4.4
1	C	193	LEU	4.4
1	C	278	VAL	4.3
1	B	201	GLN	4.3
1	A	271	ILE	4.0
1	B	143	LEU	3.9
1	C	192	ALA	3.8
1	B	76	ASP	3.6
1	C	273	GLU	3.4
1	B	225	ILE	3.4
1	A	2	ALA	3.3
1	B	307	ALA	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	251	ARG	3.3
1	C	256	THR	3.2
1	C	64	ILE	3.2
1	B	139	THR	3.2
1	A	246	ALA	3.2
1	B	158	ILE	3.2
1	C	205	GLU	3.1
1	B	204	GLU	3.1
1	B	309	LEU	3.1
1	C	269	PRO	3.1
1	B	308	GLU	3.1
1	B	189	ALA	3.0
1	C	284	ALA	3.0
1	B	168	ARG	3.0
1	B	89	LEU	3.0
1	C	215	SER	3.0
1	C	216	LEU	3.0
1	B	146	ILE	2.9
1	C	168	ARG	2.9
1	B	122	ASN	2.9
1	B	227	TYR	2.8
1	B	173	LEU	2.8
1	C	76	ASP	2.8
1	C	132	ALA	2.7
1	B	265	LEU	2.7
1	B	200	LEU	2.6
1	A	201	GLN	2.6
1	C	158	ILE	2.6
1	B	248	PHE	2.6
1	C	166	TYR	2.6
1	B	141	LEU	2.6
1	C	283	TYR	2.6
1	C	212	LEU	2.5
1	B	215	SER	2.5
1	B	177	LEU	2.5
1	B	166	TYR	2.5
1	C	33	LYS	2.5
1	B	226	LEU	2.4
1	A	205	GLU	2.4
1	B	202	MET	2.4
1	B	207	GLU	2.4
1	B	140	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	193	LEU	2.4
1	B	167	GLY	2.4
1	C	71	VAL	2.3
1	C	189	ALA	2.3
1	A	71	VAL	2.3
1	A	245	LYS	2.3
1	A	140	LEU	2.2
1	B	197	ALA	2.2
1	B	190	PRO	2.2
1	C	281	THR	2.2
1	B	109	GLN	2.1
1	C	70	SER	2.1
1	C	249	ILE	2.1
1	A	207	GLU	2.1
1	B	142	ASP	2.1
1	C	276	THR	2.0
1	A	173	LEU	2.0
1	C	294	ILE	2.0
1	A	226	LEU	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
2	PG4	A	312	13/13	0.73	0.21	53,57,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.