



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2025 – 04:06 pm BST

PDB ID : 9SQ9 / pdb\_00009sq9  
Title : Crystal Structure of the MurT/GatD Enzyme Complex from *Streptococcus pyogenes*  
Authors : Voelpel, S.V.; Stehle, T.  
Deposited on : 2025-09-19  
Resolution : 2.05 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

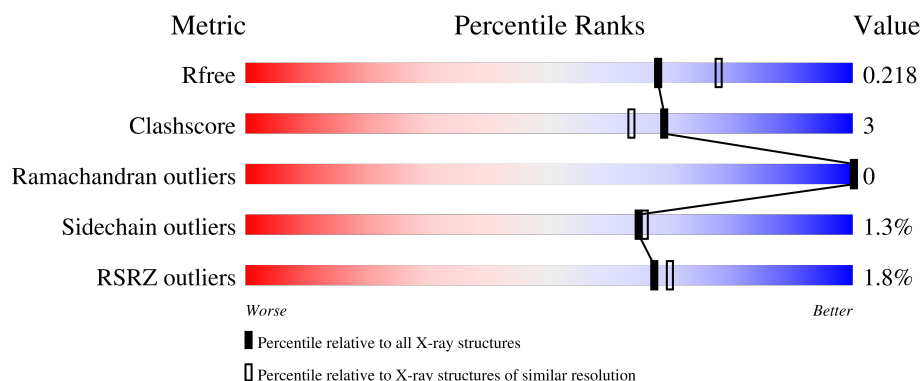
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

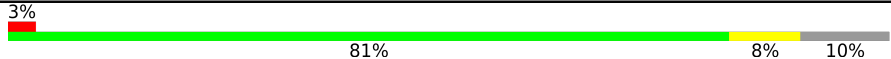

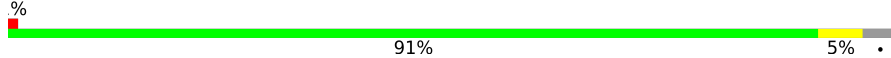

The reported resolution of this entry is 2.05 Å.

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))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	438	
1	B	438	
2	C	263	
2	D	263	

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
4	CIT	B	502	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10898 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 Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit MurT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			2990	1909	492	580	9			
1	B	406	Total	C	N	O	S	0	1	0
			3100	1981	507	600	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	HIS	-	expression tag	UNP A0A8B6J667
A	-20	HIS	-	expression tag	UNP A0A8B6J667
A	-19	HIS	-	expression tag	UNP A0A8B6J667
A	-18	HIS	-	expression tag	UNP A0A8B6J667
A	-17	HIS	-	expression tag	UNP A0A8B6J667
A	-16	HIS	-	expression tag	UNP A0A8B6J667
A	-15	PRO	-	expression tag	UNP A0A8B6J667
A	-14	MET	-	expression tag	UNP A0A8B6J667
A	-13	SER	-	expression tag	UNP A0A8B6J667
A	-12	ASP	-	expression tag	UNP A0A8B6J667
A	-11	TYR	-	expression tag	UNP A0A8B6J667
A	-10	ASP	-	expression tag	UNP A0A8B6J667
A	-9	ILE	-	expression tag	UNP A0A8B6J667
A	-8	PRO	-	expression tag	UNP A0A8B6J667
A	-7	THR	-	expression tag	UNP A0A8B6J667
A	-6	THR	-	expression tag	UNP A0A8B6J667
A	-5	GLU	-	expression tag	UNP A0A8B6J667
A	-4	ASN	-	expression tag	UNP A0A8B6J667
A	-3	LEU	-	expression tag	UNP A0A8B6J667
A	-2	TYR	-	expression tag	UNP A0A8B6J667
A	-1	PHE	-	expression tag	UNP A0A8B6J667
A	0	GLN	-	expression tag	UNP A0A8B6J667
A	1	GLY	-	expression tag	UNP A0A8B6J667
A	2	ALA	-	expression tag	UNP A0A8B6J667

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	expression tag	UNP A0A8B6J667
A	184	ARG	HIS	conflict	UNP A0A8B6J667
B	-21	HIS	-	expression tag	UNP A0A8B6J667
B	-20	HIS	-	expression tag	UNP A0A8B6J667
B	-19	HIS	-	expression tag	UNP A0A8B6J667
B	-18	HIS	-	expression tag	UNP A0A8B6J667
B	-17	HIS	-	expression tag	UNP A0A8B6J667
B	-16	HIS	-	expression tag	UNP A0A8B6J667
B	-15	PRO	-	expression tag	UNP A0A8B6J667
B	-14	MET	-	expression tag	UNP A0A8B6J667
B	-13	SER	-	expression tag	UNP A0A8B6J667
B	-12	ASP	-	expression tag	UNP A0A8B6J667
B	-11	TYR	-	expression tag	UNP A0A8B6J667
B	-10	ASP	-	expression tag	UNP A0A8B6J667
B	-9	ILE	-	expression tag	UNP A0A8B6J667
B	-8	PRO	-	expression tag	UNP A0A8B6J667
B	-7	THR	-	expression tag	UNP A0A8B6J667
B	-6	THR	-	expression tag	UNP A0A8B6J667
B	-5	GLU	-	expression tag	UNP A0A8B6J667
B	-4	ASN	-	expression tag	UNP A0A8B6J667
B	-3	LEU	-	expression tag	UNP A0A8B6J667
B	-2	TYR	-	expression tag	UNP A0A8B6J667
B	-1	PHE	-	expression tag	UNP A0A8B6J667
B	0	GLN	-	expression tag	UNP A0A8B6J667
B	1	GLY	-	expression tag	UNP A0A8B6J667
B	2	ALA	-	expression tag	UNP A0A8B6J667
B	3	MET	-	expression tag	UNP A0A8B6J667
B	184	ARG	HIS	conflict	UNP A0A8B6J667

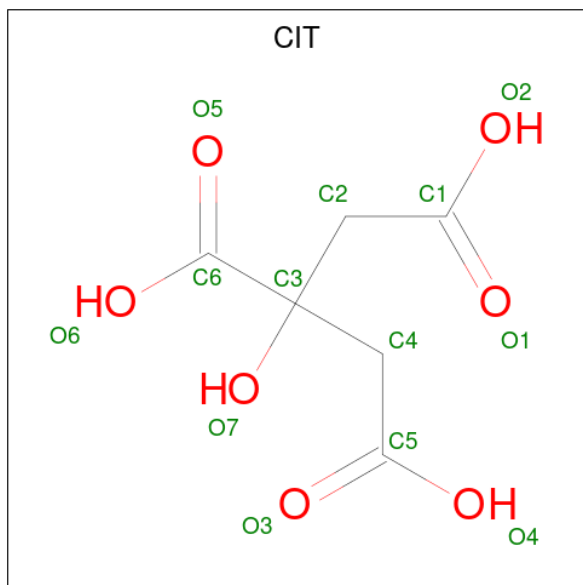
- Molecule 2 is a protein called Lipid II isoglutaminyll synthase (glutamine-hydrolyzing) subunit GatD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	253	Total	C	N	O	S	0	1	0
			1996	1270	332	390	4			
2	D	250	Total	C	N	O	S	0	2	0
			2005	1273	335	393	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

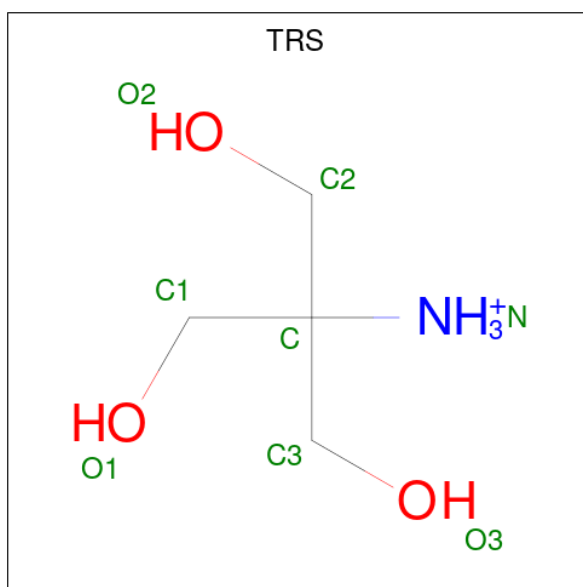
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



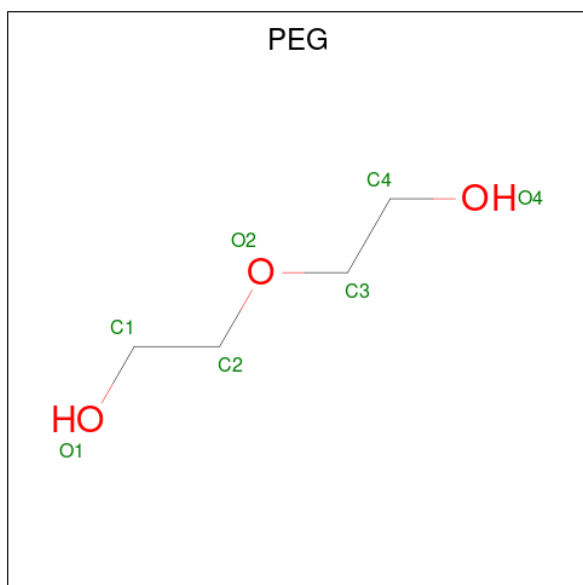
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	2	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 7 is water.

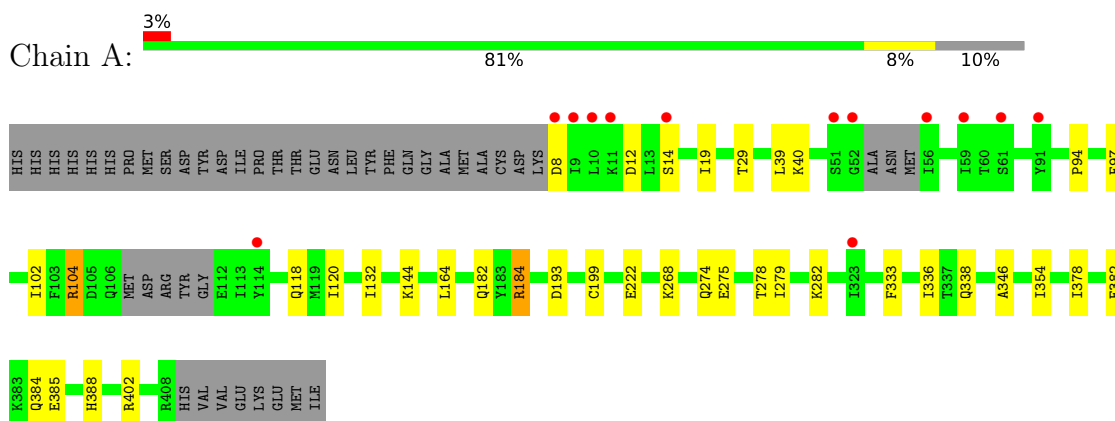
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	192	Total	O	0	0
			192	192		
7	C	143	Total	O	0	0
			143	143		
7	B	174	Total	O	0	0
			174	174		
7	D	198	Total	O	0	0
			198	198		

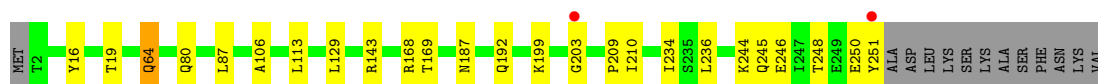


### 3 Residue-property plots

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: Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit MurT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.28Å 101.65Å 178.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 – 2.05 44.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.6 (44.14-2.05) 90.6 (44.14-2.05)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.174 , 0.218 0.177 , 0.218	Depositor DCC
$R_{free}$ test set	1838 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: CIT, ZN, TRS, PEG

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	0.55	0/3044	0.75	1/4144 (0.0%)
1	B	0.53	0/3157	0.77	1/4299 (0.0%)
2	C	0.57	0/2037	0.78	0/2759
2	D	0.59	0/2046	0.73	1/2769 (0.0%)
All	All	0.55	0/10284	0.76	3/13971 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ARG	N-CA-C	-6.01	105.94	113.28
1	B	320	ALA	N-CA-C	-5.87	106.46	113.97
2	D	19	THR	CB-CA-C	5.12	118.58	110.19

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	2990	0	2882	20	0
1	B	3100	0	3006	24	0
2	C	1996	0	1900	9	0
2	D	2005	0	1919	20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	5	1	0
4	B	13	0	5	0	0
4	C	13	0	5	0	0
4	D	13	0	5	4	0
5	A	8	0	12	0	0
5	B	24	0	36	1	0
6	B	7	0	10	0	0
6	D	7	0	10	0	0
7	A	192	0	0	4	0
7	B	174	0	0	4	0
7	C	143	0	0	3	0
7	D	198	0	0	5	0
All	All	10898	0	9795	68	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 3.

All (68) 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)
2:D:143:ARG:HH22	4:D:301:CIT:H42	1.37	0.89
1:A:29:THR:H	4:A:502:CIT:H41	1.46	0.80
1:B:375:GLU:HG3	1:B:404:LEU:HD13	1.74	0.69
1:A:118:GLN:OE1	1:A:144:LYS:NZ	2.27	0.67
1:B:319:TYR:O	7:B:601:HOH:O	2.14	0.64
2:D:245:GLN:NE2	7:D:406:HOH:O	2.33	0.61
2:D:16:TYR:OH	7:D:401:HOH:O	2.13	0.61
1:A:275:GLU:OE1	1:A:402:ARG:HD3	2.02	0.60
1:B:51:SER:HA	7:B:756:HOH:O	2.03	0.58
2:D:143:ARG:NH2	4:D:301:CIT:H42	2.16	0.57
1:B:59:ILE:HD13	1:B:88:ILE:HD13	1.86	0.55
1:B:48:THR:HG23	1:B:50:PRO:HD3	1.88	0.55
1:A:104:ARG:NH1	2:C:31[A]:TYR:OH	2.40	0.55
1:B:286:LEU:HD21	1:B:398:MET:HG3	1.88	0.54
2:C:244:LYS:O	2:C:248:THR:HG23	2.07	0.54
1:B:356[A]:ARG:NH2	7:B:602:HOH:O	2.21	0.54
1:A:333:PHE:O	1:A:336:ILE:HG12	2.07	0.54
1:A:8:ASP:N	1:A:12:ASP:H	2.06	0.53
1:A:282:LYS:NZ	1:A:384:GLN:O	2.41	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLU:HG3	1:B:263:GLY:HA2	1.91	0.52
2:C:14:TYR:CD2	2:C:50:ARG:HB2	2.45	0.51
1:B:294:GLY:HA2	5:B:505:TRS:H12	1.93	0.51
1:B:320:ALA:HB3	1:B:396:THR:HG23	1.93	0.51
2:C:50:ARG:NH1	7:C:401:HOH:O	2.29	0.50
1:B:319:TYR:C	7:B:601:HOH:O	2.55	0.50
2:D:80:GLN:HG3	2:D:113:LEU:HD11	1.92	0.50
2:D:234:ILE:HD12	2:D:236:LEU:HD21	1.94	0.50
1:A:338[A]:GLN:HE22	2:D:192:GLN:CG	2.26	0.48
1:B:34:LEU:HD11	1:B:271:PHE:CE2	2.49	0.48
2:D:168:ARG:HD2	7:D:467:HOH:O	2.14	0.47
2:C:50:ARG:HD2	7:C:401:HOH:O	2.14	0.47
1:A:388:HIS:HD2	7:A:660:HOH:O	1.98	0.46
1:B:70:LYS:HG2	1:B:74:GLN:OE1	2.14	0.46
1:A:338[A]:GLN:HE22	2:D:192:GLN:HG2	1.80	0.46
2:D:64[A]:GLN:CD	2:D:64[A]:GLN:H	2.21	0.46
2:D:210:ILE:HA	7:D:501:HOH:O	2.15	0.46
1:A:199:CYS:O	7:A:601:HOH:O	2.21	0.45
1:B:375:GLU:H	1:B:375:GLU:CD	2.25	0.45
2:D:106:ALA:O	2:D:203:GLY:HA2	2.16	0.45
2:D:143:ARG:HH12	4:D:301:CIT:H21	1.82	0.45
1:A:164:LEU:HD23	1:A:182:GLN:HG2	1.99	0.45
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.17	0.45
1:B:102:ILE:HG22	1:B:113:ILE:HG13	1.97	0.45
1:A:346:ALA:HB1	1:A:354:ILE:HG23	1.99	0.44
2:C:229:LYS:HE2	2:C:230:TYR:CZ	2.53	0.44
2:D:250:GLU:O	2:D:251:TYR:HD1	2.00	0.44
2:C:250:GLU:HG3	7:C:414:HOH:O	2.18	0.44
2:D:87:LEU:HD13	2:D:129:LEU:HG	2.00	0.43
1:A:184:ARG:HD2	1:A:193:ASP:OD2	2.17	0.43
1:B:55:MET:O	1:B:59:ILE:HD12	2.18	0.43
1:B:102:ILE:CG2	1:B:113:ILE:HG13	2.48	0.43
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.78	0.43
2:C:106:ALA:O	2:C:203:GLY:HA2	2.19	0.43
1:A:279:ILE:HD13	1:A:378:ILE:HG23	2.00	0.43
1:B:19:ILE:HB	1:B:94:PRO:HA	2.00	0.42
1:A:385:GLU:HB3	7:A:617:HOH:O	2.18	0.42
2:D:244:LYS:O	2:D:248:THR:HG23	2.19	0.42
1:A:19:ILE:HB	1:A:94:PRO:HA	2.02	0.42
1:B:346:ALA:HB1	1:B:354:ILE:HG23	2.01	0.42
1:A:222:GLU:OE2	7:A:602:HOH:O	2.22	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ARG:NH1	2:D:246:GLU:OE2	2.50	0.41
1:A:97:PHE:HB2	1:A:132:ILE:HG12	2.02	0.41
2:D:169:THR:O	2:D:187:ASN:HB3	2.21	0.41
2:C:81:SER:O	2:C:85:LYS:HG3	2.21	0.41
1:B:109:ARG:HE	4:D:301:CIT:C5	2.34	0.41
2:D:199:LYS:HE2	7:D:504:HOH:O	2.20	0.40
1:B:329:TRP:CD1	2:D:209:PRO:HD2	2.56	0.40
1:B:11:LYS:HA	1:B:91:TYR:O	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	388/438 (89%)	373 (96%)	15 (4%)	0	100	100
1	B	405/438 (92%)	392 (97%)	13 (3%)	0	100	100
2	C	252/263 (96%)	244 (97%)	8 (3%)	0	100	100
2	D	250/263 (95%)	240 (96%)	10 (4%)	0	100	100
All	All	1295/1402 (92%)	1249 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	307/374 (82%)	298 (97%)	9 (3%)	37	32
1	B	319/374 (85%)	316 (99%)	3 (1%)	75	77
2	C	207/223 (93%)	206 (100%)	1 (0%)	86	88
2	D	212/223 (95%)	210 (99%)	2 (1%)	75	77
All	All	1045/1194 (88%)	1030 (99%)	15 (1%)	65	63

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	40	LYS
1	A	102	ILE
1	A	104	ARG
1	A	120	ILE
1	A	268	LYS
1	A	274	GLN
1	A	278	THR
1	A	382	GLU
2	C	63	GLU
1	B	129	LYS
1	B	147	VAL
1	B	360	VAL
2	D	64[A]	GLN
2	D	64[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	233	ASN
1	A	297	GLN
1	A	345	ASN
2	C	59	ASN
2	C	101	ASN
2	C	120	GLN
2	C	142	ASN
1	B	74	GLN
1	B	179	HIS
1	B	182	GLN
1	B	228	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	233	ASN
1	B	239	ASN
1	B	338	GLN
2	D	12	GLN
2	D	100	ASN
2	D	116	GLN
2	D	120	GLN
2	D	142	ASN
2	D	245	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z  > 2$
5	TRS	B	505	-	7,7,7	0.32	0	9,9,9	0.49	0
4	CIT	C	301	-	12,12,12	1.28	1 (8%)	17,17,17	1.52	5 (29%)
6	PEG	B	506	-	6,6,6	0.56	0	5,5,5	0.64	0
5	TRS	B	504	-	7,7,7	0.31	0	9,9,9	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CIT	B	502	-	12,12,12	1.01	0	17,17,17	2.01	6 (35%)
4	CIT	A	502	-	12,12,12	1.16	0	17,17,17	1.92	6 (35%)
5	TRS	A	503	-	7,7,7	0.28	0	9,9,9	0.46	0
6	PEG	D	302	-	6,6,6	0.50	0	5,5,5	1.09	0
5	TRS	B	503	-	7,7,7	0.31	0	9,9,9	0.53	0
4	CIT	D	301	-	12,12,12	1.36	1 (8%)	17,17,17	2.16	6 (35%)

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
5	TRS	B	505	-	-	0/9/9/9	-
4	CIT	C	301	-	-	2/16/16/16	-
6	PEG	B	506	-	-	2/4/4/4	-
5	TRS	B	504	-	-	3/9/9/9	-
4	CIT	B	502	-	-	12/16/16/16	-
4	CIT	A	502	-	-	6/16/16/16	-
5	TRS	A	503	-	-	3/9/9/9	-
6	PEG	D	302	-	-	1/4/4/4	-
5	TRS	B	503	-	-	3/9/9/9	-
4	CIT	D	301	-	-	5/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	CIT	O7-C3	2.34	1.47	1.43
4	D	301	CIT	O3-C5	2.24	1.29	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	CIT	C4-C3-C6	-5.48	98.32	110.11
4	B	502	CIT	O6-C6-C3	4.86	121.49	113.05
4	D	301	CIT	C4-C3-C2	3.52	118.33	109.16
4	C	301	CIT	O6-C6-C3	3.47	119.08	113.05
4	A	502	CIT	C4-C3-C2	3.26	117.65	109.16
4	A	502	CIT	C4-C3-C6	-3.14	103.36	110.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	CIT	O6-C6-C3	2.93	118.14	113.05
4	D	301	CIT	O6-C6-C3	2.92	118.12	113.05
4	A	502	CIT	C2-C3-C6	-2.85	103.98	110.11
4	A	502	CIT	O2-C1-O1	-2.81	116.30	123.30
4	B	502	CIT	O4-C5-C4	2.67	122.92	114.35
4	B	502	CIT	O2-C1-C2	2.65	122.88	114.35
4	B	502	CIT	O7-C3-C6	-2.52	105.32	108.86
4	D	301	CIT	C3-C4-C5	2.50	119.88	113.81
4	D	301	CIT	O2-C1-O1	-2.43	117.24	123.30
4	D	301	CIT	O5-C6-C3	-2.35	118.93	122.25
4	B	502	CIT	O2-C1-O1	-2.33	117.49	123.30
4	C	301	CIT	C2-C3-C6	-2.33	105.10	110.11
4	A	502	CIT	O7-C3-C6	2.30	112.09	108.86
4	C	301	CIT	O2-C1-O1	-2.17	117.89	123.30
4	B	502	CIT	O3-C5-C4	-2.11	116.77	122.94
4	C	301	CIT	O4-C5-C4	2.03	120.86	114.35
4	C	301	CIT	O2-C1-C2	2.02	120.83	114.35

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	CIT	O7-C3-C6-O5
4	A	502	CIT	O7-C3-C6-O6
4	A	502	CIT	C4-C3-C6-O5
4	A	502	CIT	C4-C3-C6-O6
4	B	502	CIT	O7-C3-C6-O5
4	B	502	CIT	O7-C3-C6-O6
4	B	502	CIT	C4-C3-C6-O5
4	B	502	CIT	C4-C3-C6-O6
4	D	301	CIT	C1-C2-C3-O7
4	D	301	CIT	C1-C2-C3-C4
4	D	301	CIT	C1-C2-C3-C6
5	B	503	TRS	C1-C-C2-O2
5	B	503	TRS	C3-C-C2-O2
5	B	504	TRS	C1-C-C2-O2
5	B	504	TRS	N-C-C2-O2
4	B	502	CIT	C1-C2-C3-O7
4	A	502	CIT	C1-C2-C3-C4
4	B	502	CIT	C1-C2-C3-C4
4	A	502	CIT	C1-C2-C3-O7
4	B	502	CIT	C1-C2-C3-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	B	506	PEG	O2-C3-C4-O4
6	D	302	PEG	O1-C1-C2-O2
5	A	503	TRS	C1-C-C2-O2
5	A	503	TRS	N-C-C2-O2
5	B	504	TRS	C3-C-C2-O2
6	B	506	PEG	C1-C2-O2-C3
4	B	502	CIT	C2-C3-C6-O5
4	B	502	CIT	C2-C3-C6-O6
4	C	301	CIT	C1-C2-C3-O7
4	B	502	CIT	C2-C3-C4-C5
5	A	503	TRS	C3-C-C2-O2
4	B	502	CIT	C3-C4-C5-O4
4	D	301	CIT	C3-C4-C5-O4
4	B	502	CIT	C3-C4-C5-O3
4	D	301	CIT	C3-C4-C5-O3
4	C	301	CIT	C1-C2-C3-C6
5	B	503	TRS	N-C-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	TRS	1	0
4	A	502	CIT	1	0
4	D	301	CIT	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	393/438 (89%)	-0.05	13 (3%)	49	51	21, 43, 72, 97	1 (0%)
1	B	406/438 (92%)	-0.17	6 (1%)	71	74	20, 43, 69, 85	2 (0%)
2	C	253/263 (96%)	-0.36	2 (0%)	82	85	19, 36, 58, 85	1 (0%)
2	D	250/263 (95%)	-0.54	2 (0%)	82	85	16, 33, 47, 79	3 (1%)
All	All	1302/1402 (92%)	-0.24	23 (1%)	67	70	16, 39, 66, 97	7 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ILE	6.6
1	A	8	ASP	4.9
1	A	10	LEU	4.9
1	B	319	TYR	4.0
1	A	114	TYR	3.9
1	B	114	TYR	3.8
1	A	91	TYR	3.7
2	D	251	TYR	3.5
2	C	31[A]	TYR	3.4
1	B	2	ALA	3.4
1	A	14	SER	3.3
1	B	320	ALA	3.0
2	C	254	LEU	3.0
1	A	11	LYS	3.0
1	B	4	ALA	2.7
2	D	203	GLY	2.6
1	A	51	SER	2.4
1	A	61	SER	2.4
1	A	59	ILE	2.4
1	B	113	ILE	2.4
1	A	52	GLY	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	323	ILE	2.1
1	A	56	ILE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
5	TRS	A	503	8/8	0.67	0.14	59,73,80,80	0
5	TRS	B	504	8/8	0.75	0.12	71,79,86,90	0
4	CIT	D	301	13/13	0.81	0.14	45,59,71,75	0
5	TRS	B	503	8/8	0.82	0.14	51,65,77,78	0
4	CIT	B	502	13/13	0.82	0.11	44,66,80,89	0
4	CIT	A	502	13/13	0.84	0.12	41,47,59,69	5
5	TRS	B	505	8/8	0.84	0.15	56,61,67,71	0
6	PEG	B	506	7/7	0.84	0.14	45,51,60,64	0
6	PEG	D	302	7/7	0.85	0.14	49,52,66,68	0
4	CIT	C	301	13/13	0.92	0.10	38,48,56,58	0
3	ZN	A	501	1/1	0.99	0.02	39,39,39,39	0
3	ZN	B	501	1/1	1.00	0.02	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.