



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:11 PM GMT

PDB ID : 4R40  
Title : Crystal Structure of TolB/Pal complex from Yersinia pestis.  
Authors : Maltseva, N.; Kim, Y.; Osipiuk, J.; Anderson, W.F.; Joachimiak, A.; Center  
for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2014-08-18  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

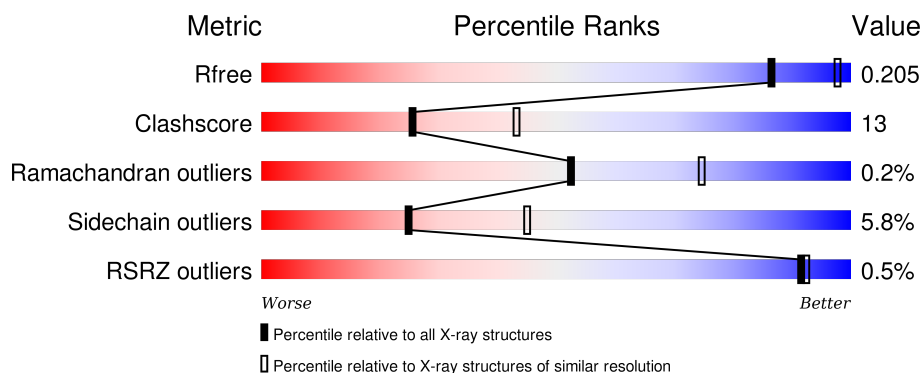
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	411	<div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	C	411	<div> <div>71%</div> <div>24%</div> <div>..</div> </div>
2	B	141	<div> <div>68%</div> <div>17%</div> <div>•</div> <div>12%</div> </div>
2	D	141	<div> <div>65%</div> <div>20%</div> <div>..</div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8156 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 Protein TolB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	Se	0	2	0
			3079	1941	533	599	6			
1	C	405	Total	C	N	O	Se	0	1	0
			3063	1931	531	596	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	-	EXPRESSION TAG	UNP Q8ZGZ1
A	21	ASN	-	EXPRESSION TAG	UNP Q8ZGZ1
A	22	ALA	-	EXPRESSION TAG	UNP Q8ZGZ1
C	20	SER	-	EXPRESSION TAG	UNP Q8ZGZ1
C	21	ASN	-	EXPRESSION TAG	UNP Q8ZGZ1
C	22	ALA	-	EXPRESSION TAG	UNP Q8ZGZ1

- Molecule 2 is a protein called Peptidoglycan-associated lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	Se	0	0	0
			967	604	172	188	3			
2	D	124	Total	C	N	O	Se	0	0	0
			967	604	172	188	3			

There are 6 discrepancies between the modelled and reference sequences:

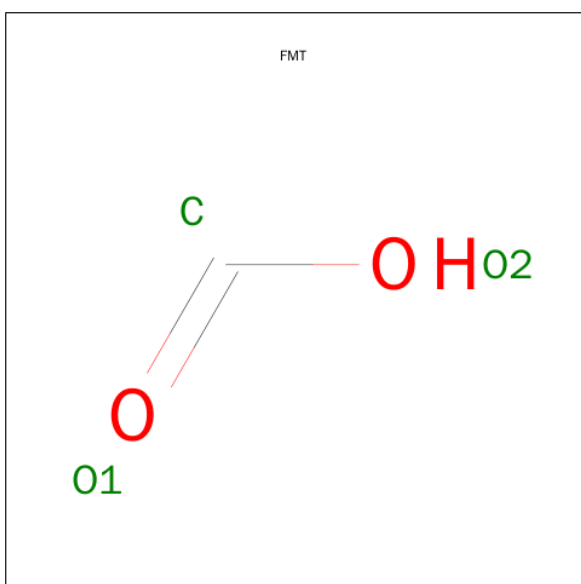
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	SER	-	EXPRESSION TAG	UNP Q7CH55
B	29	ASN	-	EXPRESSION TAG	UNP Q7CH55
B	30	ALA	-	EXPRESSION TAG	UNP Q7CH55
D	28	SER	-	EXPRESSION TAG	UNP Q7CH55
D	29	ASN	-	EXPRESSION TAG	UNP Q7CH55
D	30	ALA	-	EXPRESSION TAG	UNP Q7CH55

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	7	Total	O	0	0
			7	7		
6	C	12	Total	O	0	0
			12	12		
6	D	3	Total	O	0	0
			3	3		





● Molecule 2: Peptidoglycan-associated lipoprotein



SER	ASN	ALA	ASP	GLN	SER	GLY	PSE	GLY	ALA	GLY	THR	GLY	THR	GLU	ASN	GLY	S45	S49	M57	D74	D78	L90	D96	V100	A104	D105	E106	T109	P110	E111	Y112	M113	E118	R119	R120	V124	V133	D136	Q137	I140	K145	E146	K147	P148
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.39Å 175.25Å 66.27Å 90.00° 89.83° 90.00°	Depositor
Resolution (Å)	43.82 – 2.50 43.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.2 (43.82-2.50) 80.8 (43.82-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, $R_{free}$	0.170 , 0.214 0.170 , 0.205	Depositor DCC
$R_{free}$ test set	1550 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.0	EDS
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30433 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, FMT, SO4

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	0.44	3/3146 (0.1%)	0.54	4/4281 (0.1%)
1	C	0.42	4/3130 (0.1%)	0.53	5/4259 (0.1%)
2	B	0.40	1/980 (0.1%)	0.47	1/1313 (0.1%)
2	D	0.33	0/980	0.42	0/1313
All	All	0.42	8/8236 (0.1%)	0.51	10/11166 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	PRO	N-CD	5.36	1.55	1.47
1	A	428	PRO	N-CD	5.31	1.55	1.47
1	C	80	PRO	N-CD	5.30	1.55	1.47
2	B	110	PRO	N-CD	5.29	1.55	1.47
1	A	201	PRO	N-CD	5.21	1.55	1.47
1	C	201	PRO	N-CD	5.17	1.55	1.47
1	A	380	PRO	N-CD	5.16	1.55	1.47
1	C	380	PRO	N-CD	5.06	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	PHE	C-N-CD	5.75	140.48	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	379	THR	C-N-CD	5.65	140.27	128.40
1	C	423	PHE	C-N-CD	5.63	140.22	128.40
1	A	427	SER	C-N-CD	5.55	140.06	128.40
2	B	109	THR	C-N-CD	5.49	139.92	128.40
1	A	379	THR	C-N-CD	5.46	139.87	128.40
1	A	200	GLU	C-N-CD	5.45	139.85	128.40
1	C	79	GLN	C-N-CD	5.45	139.85	128.40
1	C	200	GLU	C-N-CD	5.45	139.85	128.40
1	C	242	PHE	C-N-CD	5.30	139.53	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	162	ARG	Sidechain

## 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	3079	0	3020	85	0
1	C	3063	0	3002	80	0
2	B	967	0	943	21	0
2	D	967	0	943	23	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	3	0	1	0	0
4	B	3	0	1	0	0
5	B	12	0	16	1	0
5	C	6	0	8	0	0
6	A	14	0	0	0	0
6	B	7	0	0	0	0
6	C	12	0	0	0	0
6	D	3	0	0	0	0
All	All	8156	0	7934	201	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 13.

All (201) 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:273[A]:MSE:HE3	1:A:278:GLY:HA2	1.56	0.88
2:D:105:ASP:HB2	2:D:158:PHE:CD1	2.15	0.80
1:C:422:LYS:HG3	1:C:423:PHE:HD2	1.48	0.79
1:A:277:SER:OG	1:A:279:GLN:HG3	1.84	0.78
1:C:365:THR:HG21	1:C:367:ALA:HB2	1.67	0.76
2:D:96:ASP:O	2:D:137:GLN:HG2	1.86	0.76
1:C:160:LYS:HD3	1:C:429:TYR:CE1	2.23	0.73
1:A:248:ALA:HB2	2:B:111:GLU:HG2	1.70	0.73
2:B:139:SER:HB3	5:B:203:GOL:H2	1.70	0.73
1:C:200:GLU:HG3	1:C:201:PRO:HD2	1.73	0.71
1:A:378:GLU:OE2	2:B:110:PRO:HD3	1.91	0.70
1:A:78:GLN:HE22	1:A:86:VAL:HA	1.57	0.69
1:A:422:LYS:HB3	1:A:423:PHE:CD2	2.27	0.69
1:C:38:GLY:HA2	1:C:71:ILE:HG22	1.75	0.68
1:C:365:THR:CG2	1:C:367:ALA:HB2	2.24	0.67
1:C:422:LYS:HE3	1:C:423:PHE:CE2	2.31	0.66
1:C:213:LYS:HG2	1:C:230:THR:HG22	1.77	0.66
2:D:136:ASP:OD1	2:D:136:ASP:N	2.28	0.66
1:A:243:PRO:O	1:A:244:ARG:HB2	1.97	0.64
1:C:25:ILE:HD11	1:C:188:ASP:HA	1.78	0.64
1:C:160:LYS:HD3	1:C:429:TYR:CZ	2.33	0.64
1:A:248:ALA:HB1	1:A:293:PRO:HD2	1.80	0.63
1:C:301:ASN:OD1	1:C:318:ASN:ND2	2.31	0.63
1:A:205:PRO:HD2	1:A:423:PHE:HB3	1.80	0.63
1:C:213:LYS:HE3	1:C:230:THR:HG22	1.80	0.63
2:B:97:LYS:HG3	2:B:137:GLN:HA	1.81	0.63
1:C:378:GLU:HG3	1:C:392:SER:HB2	1.80	0.63
1:A:422:LYS:HB3	1:A:423:PHE:HD2	1.64	0.62
1:A:379:THR:O	1:A:379:THR:HG22	2.00	0.62
1:A:336:ASN:HB2	2:B:109:THR:HG21	1.82	0.61
1:C:269:ASN:HB2	1:C:271:TYR:HE1	1.65	0.61
1:A:202:LEU:HD22	1:A:216:TYR:CE1	2.36	0.61
1:A:78:GLN:HE21	1:A:91:TRP:HE1	1.47	0.61
2:D:109:THR:O	2:D:113:ASN:ND2	2.33	0.61
2:D:149:ALA:N	2:D:161:ASN:OD1	2.34	0.61
1:C:150:ASP:OD2	1:C:164:ARG:NE	2.35	0.60
1:C:82:THR:HG22	1:C:85:GLU:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:HB2	1:A:129:LEU:HD11	1.84	0.59
1:C:80:PRO:HG3	1:C:86:VAL:HG22	1.83	0.59
1:A:226:LEU:HD22	1:A:239:VAL:CG2	2.32	0.59
1:A:377:ASP:OD1	1:A:391:TYR:HE1	1.85	0.59
1:C:316:LYS:HB2	1:C:327:ILE:HD13	1.85	0.58
1:A:196:HIS:NE2	1:A:220:GLU:OE2	2.36	0.58
1:C:76:MSE:HE2	1:C:79:GLN:HG2	1.85	0.58
1:C:228:ILE:HG13	1:C:239:VAL:HG11	1.86	0.58
1:C:76:MSE:CE	1:C:79:GLN:HG2	2.34	0.58
1:A:82:THR:HG23	1:A:84:ALA:H	1.67	0.58
1:A:358:ILE:HB	1:A:372:THR:HG23	1.85	0.57
2:B:70:PHE:O	2:B:71:ASP:HB2	2.03	0.57
1:C:213:LYS:HE3	1:C:230:THR:CG2	2.35	0.57
1:A:80:PRO:HB3	1:A:85:GLU:HB2	1.87	0.56
1:A:118:LEU:HG	1:A:129:LEU:HD13	1.87	0.56
1:C:377:ASP:HA	1:C:392:SER:O	2.06	0.56
1:A:196:HIS:HD2	1:A:202:LEU:HD21	1.71	0.56
1:A:224:SER:OG	1:A:245:HIS:HA	2.06	0.56
1:C:80:PRO:HB2	1:C:85:GLU:HB2	1.88	0.56
2:B:75:ILE:HD11	2:B:124:VAL:HA	1.87	0.55
1:C:180:HIS:CE1	1:C:199:PRO:O	2.59	0.55
1:A:333:GLN:HG2	1:A:335:GLN:HE21	1.71	0.55
1:A:132:ASN:OD1	1:A:133:GLN:N	2.39	0.55
1:A:78:GLN:NE2	1:A:91:TRP:HE1	2.03	0.55
1:C:44:TRP:CH2	1:C:106:PRO:HG3	2.42	0.55
1:A:287:ARG:HB2	1:C:266:GLY:HA3	1.88	0.55
1:A:326:ARG:NE	1:A:328:THR:O	2.33	0.54
1:A:226:LEU:HD22	1:A:239:VAL:HG21	1.88	0.54
1:A:34:ALA:O	1:A:36:PRO:HD3	2.07	0.54
2:D:78:ASP:OD1	2:D:78:ASP:N	2.36	0.54
1:C:312:PRO:HD2	1:C:333:GLN:HG3	1.90	0.53
1:A:292:GLU:OE2	2:B:109:THR:OG1	2.22	0.53
1:C:290:ASN:HB3	1:C:304:TYR:CE1	2.43	0.53
2:D:100:VAL:HB	2:D:140:ILE:HG22	1.90	0.53
1:A:210:ASP:OD1	1:A:211:GLY:N	2.37	0.53
1:A:358:ILE:HB	1:A:372:THR:CG2	2.39	0.52
1:A:171:VAL:HG22	1:A:421:VAL:HG22	1.91	0.52
1:C:42:PHE:CD2	1:C:102:GLY:HA3	2.46	0.51
1:C:422:LYS:HE3	1:C:423:PHE:HE2	1.73	0.51
1:C:274:ASP:HB3	1:C:277:SER:OG	2.09	0.51
1:A:111:SER:OG	1:A:135:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:HIS:HE1	1:C:199:PRO:O	1.94	0.51
1:C:273:MSE:HE3	1:C:278:GLY:HA2	1.92	0.51
1:A:391:TYR:CE2	1:A:402:GLN:HB2	2.46	0.51
1:C:77:PRO:HD3	1:C:94:LEU:HD12	1.92	0.50
1:C:118:LEU:HD22	1:C:152:VAL:HG22	1.93	0.50
1:A:358:ILE:HG12	1:A:377:ASP:HB3	1.92	0.50
1:A:337:ALA:HB1	1:A:346:LEU:HD22	1.93	0.50
1:A:310:GLY:O	1:A:311:ARG:C	2.50	0.50
2:B:73:TYR:CZ	2:B:119:ARG:HD2	2.47	0.50
1:A:373:ASP:OD1	1:A:373:ASP:N	2.45	0.49
2:B:155:GLU:OE2	2:B:162:ARG:NH2	2.39	0.49
2:D:106:GLU:HA	2:D:145:LYS:HD2	1.93	0.49
1:C:42:PHE:N	1:C:42:PHE:CD1	2.81	0.49
1:A:243:PRO:O	1:A:244:ARG:CB	2.60	0.49
1:A:117:GLN:HE21	1:A:131:GLN:NE2	2.11	0.49
1:C:314:VAL:HB	1:C:328:THR:CG2	2.43	0.48
2:B:157:ALA:O	2:B:161:ASN:ND2	2.46	0.48
1:A:37:ILE:HG13	1:A:38:GLY:N	2.28	0.48
1:A:377:ASP:OD1	1:A:391:TYR:CE1	2.64	0.48
1:C:298:ASP:OD2	1:C:301:ASN:ND2	2.47	0.48
2:B:116:LEU:O	2:B:120:ARG:HG3	2.14	0.48
2:B:73:TYR:HB2	2:B:120:ARG:HG2	1.95	0.48
1:C:96:ILE:O	1:C:121:THR:OG1	2.27	0.48
1:C:422:LYS:HG3	1:C:423:PHE:CD2	2.37	0.48
1:C:165:THR:HG21	1:C:426:TRP:CD1	2.49	0.48
1:C:44:TRP:CG	1:C:50:PRO:HG3	2.49	0.47
1:C:42:PHE:N	1:C:42:PHE:HD1	2.11	0.47
2:D:104:ALA:O	2:D:145:LYS:HA	2.14	0.47
1:A:62:LEU:HB3	1:A:68:PHE:HB2	1.95	0.47
1:C:378:GLU:HG3	1:C:392:SER:CB	2.45	0.47
1:A:388:MSE:HG3	1:A:389:VAL:N	2.29	0.47
1:C:356:GLN:HE21	1:C:376:LEU:HD22	1.80	0.47
1:A:227:VAL:HG12	1:A:238:GLN:HA	1.95	0.47
1:C:292:GLU:N	1:C:293:PRO:CD	2.78	0.47
2:D:145:LYS:CG	2:D:146:GLU:OE1	2.63	0.47
1:C:118:LEU:O	1:C:129:LEU:N	2.45	0.47
1:A:246:ASN:N	1:A:246:ASN:ND2	2.63	0.47
2:B:140:ILE:HG13	2:B:140:ILE:O	2.15	0.47
1:A:323:VAL:O	1:A:325:GLN:NE2	2.40	0.47
1:A:203:MSE:HB2	1:A:217:VAL:HG22	1.97	0.47
2:D:106:GLU:HB2	2:D:158:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PRO:HD2	1:A:299:SER:OG	2.15	0.46
1:C:314:VAL:HB	1:C:328:THR:HG23	1.97	0.46
2:D:145:LYS:HG2	2:D:146:GLU:OE1	2.15	0.46
1:C:248:ALA:HB1	1:C:293:PRO:HD2	1.97	0.46
1:C:26:GLU:HG2	1:C:415:PRO:HD3	1.98	0.46
2:D:154:ASP:O	2:D:158:PHE:N	2.33	0.46
2:B:125:LYS:HE2	2:B:138:ILE:HB	1.98	0.46
1:A:304:TYR:OH	1:A:324:PRO:HB3	2.15	0.46
1:C:244:ARG:HB2	1:C:245:HIS:H	1.58	0.45
1:A:147:THR:HA	1:A:164:ARG:HD3	1.99	0.45
1:C:422:LYS:HE3	1:C:423:PHE:CD2	2.52	0.45
2:B:150:VAL:HB	2:B:157:ALA:HA	1.99	0.45
1:C:183:ARG:HD3	1:C:192:GLN:HE21	1.82	0.45
2:B:154:ASP:N	2:B:154:ASP:OD1	2.47	0.45
1:C:204:SER:HB3	1:C:249:PRO:HD2	1.99	0.45
1:A:270:LEU:H	1:A:284:THR:HB	1.82	0.45
1:C:263:SER:OG	2:D:118:GLU:OE2	2.31	0.45
1:A:45:MSE:HG3	1:A:105:GLN:HG2	1.99	0.45
2:D:104:ALA:HA	2:D:120:ARG:HH12	1.82	0.44
1:C:80:PRO:CB	1:C:85:GLU:HB2	2.46	0.44
1:C:44:TRP:CH2	1:C:51:PRO:HD3	2.53	0.44
1:C:249:PRO:HA	1:C:259:ALA:O	2.17	0.44
2:D:57:MSE:HE1	2:D:168:TYR:CZ	2.52	0.44
1:C:105:GLN:HA	1:C:106:PRO:HD3	1.86	0.44
1:C:49:THR:HA	1:C:50:PRO:HD3	1.87	0.44
1:A:139:GLN:OE1	1:A:140:TRP:CZ3	2.70	0.44
2:D:154:ASP:H	2:D:157:ALA:HB3	1.82	0.44
1:A:24:ARG:HH22	1:A:57:ILE:HG12	1.83	0.44
2:D:100:VAL:HG11	2:D:124:VAL:HB	2.00	0.43
1:C:300:GLN:HG2	1:C:318:ASN:ND2	2.33	0.43
1:C:77:PRO:HD3	1:C:94:LEU:CD1	2.48	0.43
1:C:118:LEU:HB3	1:C:130:ALA:H	1.83	0.43
1:C:43:LYS:HG2	1:C:45:MSE:SE	2.68	0.43
1:A:282:GLN:NE2	1:A:284:THR:O	2.33	0.43
1:A:181:GLU:HG2	1:A:197:ARG:HG2	2.00	0.43
1:A:289:ASN:HB2	1:A:307:ASP:OD1	2.18	0.43
1:A:292:GLU:HG3	2:B:111:GLU:HB3	1.99	0.43
1:C:42:PHE:CE2	1:C:102:GLY:HA3	2.54	0.43
1:A:379:THR:HG21	1:A:423:PHE:HA	2.00	0.43
1:A:388:MSE:HB2	1:A:388:MSE:HE2	1.73	0.43
1:A:418:ASP:HB3	1:A:419:GLY:H	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASN:ND2	1:C:306:SER:OG	2.52	0.43
1:A:59:GLY:O	1:A:70:PRO:HG2	2.19	0.43
2:D:106:GLU:HB2	2:D:158:PHE:CE1	2.54	0.42
1:A:291:THR:OG1	1:A:292:GLU:N	2.52	0.42
1:C:248:ALA:N	2:D:111:GLU:OE2	2.53	0.42
1:A:42:PHE:CE2	1:A:102:GLY:HA3	2.55	0.42
1:C:160:LYS:CD	1:C:429:TYR:CZ	3.02	0.42
2:B:149:ALA:N	2:B:161:ASN:OD1	2.42	0.42
1:C:226:LEU:HD11	1:C:249:PRO:HB3	2.01	0.42
1:A:202:LEU:HD22	1:A:216:TYR:HE1	1.79	0.42
1:A:273[A]:MSE:CE	1:A:278:GLY:HA2	2.40	0.42
1:A:226:LEU:HD23	1:A:227:VAL:N	2.34	0.42
1:A:111:SER:HA	1:A:137:THR:HA	2.02	0.42
1:A:166:ARG:HG3	1:A:430:LEU:HD11	2.02	0.42
1:A:78:GLN:HE22	1:A:87:THR:H	1.66	0.42
1:C:270:LEU:HD11	1:C:304:TYR:CG	2.54	0.42
1:C:363:LEU:HD23	1:C:363:LEU:HA	1.71	0.42
2:B:73:TYR:CB	2:B:120:ARG:HG2	2.49	0.41
1:C:61:ASP:OD1	1:C:187:TYR:OH	2.37	0.41
1:C:82:THR:HG23	1:C:84:ALA:H	1.85	0.41
1:A:247:GLY:O	1:A:260:PHE:HB2	2.20	0.41
1:A:34:ALA:HB3	1:A:69:ASN:HB2	2.02	0.41
1:C:248:ALA:O	1:C:260:PHE:HA	2.20	0.41
2:B:131:LYS:HA	2:B:131:LYS:HD3	1.82	0.41
2:D:149:ALA:HB2	2:D:163:ARG:CZ	2.51	0.41
1:C:165:THR:HG22	1:C:166:ARG:O	2.20	0.41
2:D:105:ASP:OD2	2:D:162:ARG:NH2	2.54	0.41
2:D:90:LEU:HD13	2:D:133:VAL:HG11	2.02	0.41
1:A:165:THR:HG21	1:A:384:PRO:HG3	2.03	0.41
1:A:277:SER:CB	1:A:279:GLN:HG3	2.51	0.41
1:C:100:VAL:HG22	1:C:118:LEU:HD13	2.02	0.41
1:C:166:ARG:HG3	1:C:186:ASP:HA	2.01	0.41
1:A:307:ASP:N	1:A:307:ASP:OD1	2.54	0.41
1:C:357:HIS:HA	1:C:377:ASP:OD2	2.21	0.41
1:A:107:SER:OG	1:A:108:ALA:N	2.53	0.40
1:A:196:HIS:CD2	1:A:202:LEU:HD21	2.53	0.40
1:C:165:THR:HG23	1:C:427:SER:OG	2.21	0.40
1:A:252:SER:O	1:A:255:GLY:N	2.51	0.40
1:A:296:PHE:CZ	1:A:316:LYS:HD2	2.57	0.40
1:A:169:TYR:OH	1:A:192:GLN:HG3	2.21	0.40
1:A:198:SER:HA	1:A:199:PRO:HD3	1.90	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	404/411 (98%)	394 (98%)	8 (2%)	2 (0%)	34	55
1	C	402/411 (98%)	395 (98%)	7 (2%)	0	100	100
2	B	122/141 (86%)	121 (99%)	1 (1%)	0	100	100
2	D	122/141 (86%)	117 (96%)	5 (4%)	0	100	100
All	All	1050/1104 (95%)	1027 (98%)	21 (2%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	244	ARG

### 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	333/329 (101%)	316 (95%)	17 (5%)	29	52
1	C	330/329 (100%)	310 (94%)	20 (6%)	23	42
2	B	100/106 (94%)	95 (95%)	5 (5%)	30	53
2	D	100/106 (94%)	92 (92%)	8 (8%)	15	28
All	All	863/870 (99%)	813 (94%)	50 (6%)	25	45

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	97	ASP
1	A	107	SER
1	A	133	GLN
1	A	187	TYR
1	A	217	VAL
1	A	241	SER
1	A	246	ASN
1	A	257	LYS
1	A	258	LEU
1	A	265	SER
1	A	275	LEU
1	A	285	ASP
1	A	317	VAL
1	A	378	GLU
1	A	387	THR
1	A	427	SER
2	B	46	ASN
2	B	62	LYS
2	B	70	PHE
2	B	71	ASP
2	B	134	SER
1	C	24	ARG
1	C	135	LYS
1	C	154	GLU
1	C	155	LYS
1	C	166	ARG
1	C	202	LEU
1	C	203	MSE
1	C	237	ARG
1	C	239	VAL
1	C	241	SER
1	C	244	ARG
1	C	271	TYR
1	C	274	ASP
1	C	275	LEU
1	C	299	SER
1	C	378	GLU
1	C	382	ILE
1	C	393	SER
1	C	422	LYS
1	C	427	SER

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Mol	Chain	Res	Type
2	D	45	SER
2	D	49	SER
2	D	57	MSE
2	D	74	ASP
2	D	136	ASP
2	D	146	GLU
2	D	147	LYS
2	D	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	131	GLN
1	A	133	GLN
1	A	180	HIS
1	A	191	ASN
1	A	334	ASN
1	A	335	GLN
1	A	336	ASN
1	A	402	GLN
2	B	113	ASN
1	C	192	GLN
1	C	269	ASN
1	C	279	GLN
1	C	290	ASN
1	C	308	GLN
1	C	333	GLN
2	D	58	GLN
2	D	129	GLN

### 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

9 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	$\# Z  > 2$
3	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.07	0
4	FMT	A	502	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	201	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	202	-	5,5,5	0.33	0	5,5,5	0.21	0
5	GOL	B	203	-	5,5,5	0.35	0	5,5,5	0.22	0
3	SO4	B	204	-	4,4,4	0.80	0	6,6,6	0.18	0
5	GOL	C	501	-	5,5,5	0.34	0	5,5,5	0.24	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	201	-	4,4,4	0.13	0	6,6,6	0.11	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
4	FMT	A	502	-	-	0/0/0/0	0/0/0/0
4	FMT	B	201	-	-	0/0/0/0	0/0/0/0
5	GOL	B	202	-	-	0/4/4/4	0/0/0/0
5	GOL	B	203	-	-	0/4/4/4	0/0/0/0
3	SO4	B	204	-	-	0/0/0/0	0/0/0/0
5	GOL	C	501	-	-	0/4/4/4	0/0/0/0
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
3	SO4	D	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	203	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	401/411 (97%)	-0.42	2 (0%) 91 92	27, 43, 64, 87	9 (2%)
1	C	400/411 (97%)	-0.41	2 (0%) 91 92	28, 45, 64, 81	10 (2%)
2	B	121/141 (85%)	-0.47	0 100 100	30, 43, 66, 82	9 (7%)
2	D	121/141 (85%)	-0.41	1 (0%) 87 89	30, 44, 64, 70	7 (5%)
All	All	1043/1104 (94%)	-0.42	5 (0%) 91 92	27, 44, 64, 87	35 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	VAL	8.3
1	A	125	ALA	3.0
1	C	342	ASP	2.9
2	D	153	HIS	2.6
1	C	109	ASP	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 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(Å <sup>2</sup> )	Q<0.9
3	SO4	D	201	5/5	0.96	0.23	2.71	17,25,29,31	5
5	GOL	B	203	6/6	0.96	0.14	1.55	22,47,56,57	0
4	FMT	A	502	3/3	0.96	0.15	0.86	58,58,60,63	0
3	SO4	C	502	5/5	0.95	0.14	0.72	43,54,58,63	5
5	GOL	B	202	6/6	0.94	0.13	-0.07	32,49,51,54	0
3	SO4	B	204	5/5	1.00	0.10	-0.79	23,29,35,37	0
4	FMT	B	201	3/3	0.98	0.10	-1.01	42,42,49,54	0
5	GOL	C	501	6/6	0.96	0.08	-1.58	44,46,50,51	0
3	SO4	A	501	5/5	0.97	0.09	-	73,79,85,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.