



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:33 pm GMT

PDB ID : 2Q9A  
Title : Structure of Apo FTSY  
Authors : Reyes, C.L.; Stroud, R.M.  
Deposited on : 2007-06-12  
Resolution : 2.24 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.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

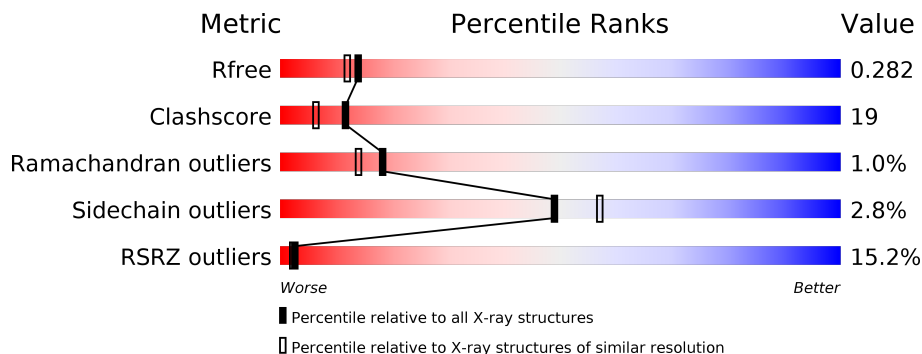
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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	304	
1	B	304	

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
2	SO4	A	752	-	-	-	X
3	EDO	A	900	-	-	-	X
3	EDO	A	901	-	-	-	X
3	EDO	A	906	-	-	-	X
3	EDO	A	908	-	-	-	X
3	EDO	B	903	-	-	-	X
3	EDO	B	904	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5008 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 Cell division protein ftsY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2327	1485	405	430	7			
1	B	290	Total	C	N	O	S	0	0	0
			2209	1412	379	411	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



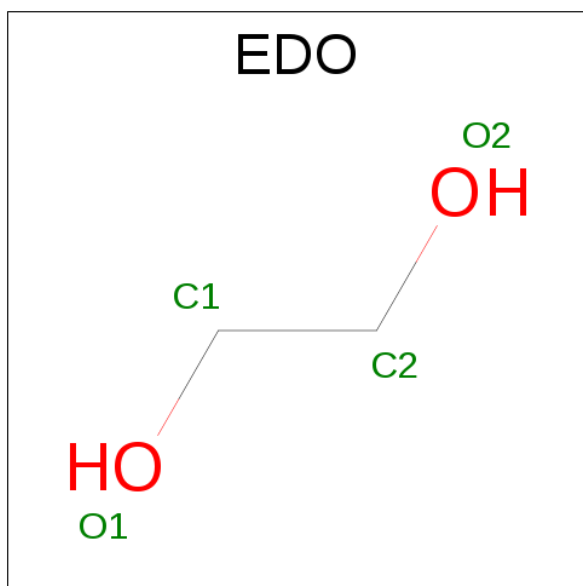
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

Continued on next page...

*Continued from previous page...*

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

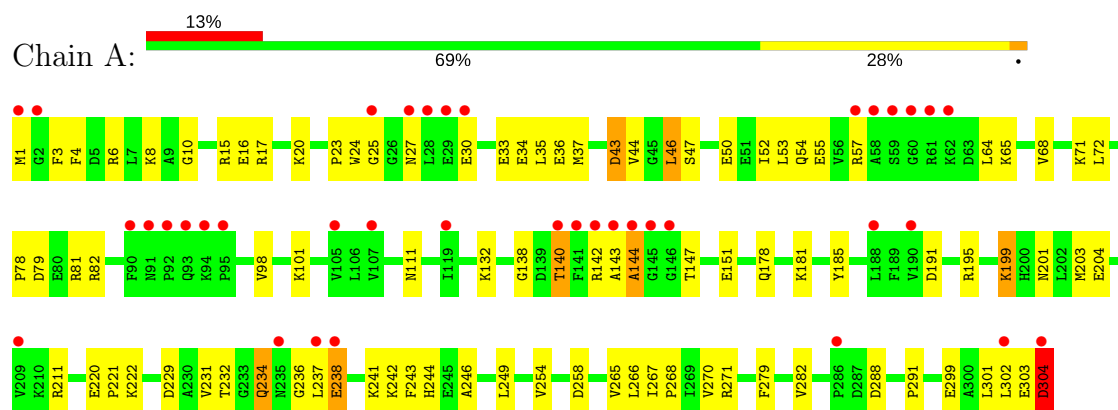
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	212	Total O 212 212	0	0
4	B	179	Total O 179 179	0	0

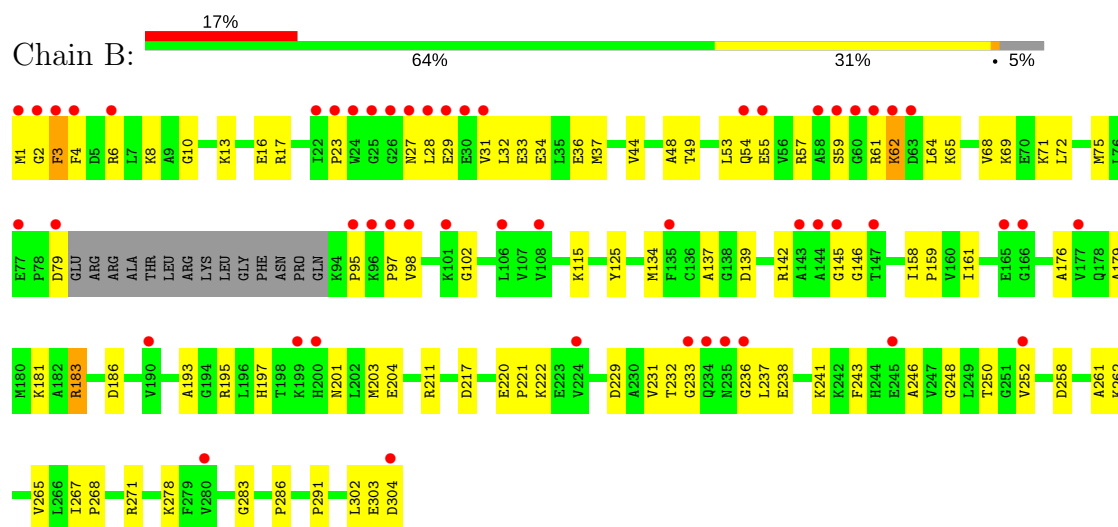
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Cell division protein ftsY



#### • Molecule 1: Cell division protein ftsY



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.63Å 96.68Å 99.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.24 19.70 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.70-2.24) 99.3 (19.70-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.84 (at 2.26Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.223 , 0.247 0.263 , 0.282	Depositor DCC
$R_{free}$ test set	2839 reflections (9.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: SO4, EDO

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	0.93	1/2365 (0.0%)	0.86	2/3189 (0.1%)
1	B	0.89	1/2244 (0.0%)	0.87	4/3026 (0.1%)
All	All	0.91	2/4609 (0.0%)	0.86	6/6215 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	PHE	CE2-CZ	5.16	1.47	1.37
1	B	252	VAL	CB-CG2	-5.01	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	183	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	186	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	79	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	304	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	140	THR	OG1-CB-CG2	-5.01	98.48	110.00

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	2327	0	2425	97	0
1	B	2209	0	2299	92	0
2	A	25	0	0	1	0
2	B	20	0	0	0	0
3	A	24	0	36	5	0
3	B	12	0	18	5	0
4	A	212	0	0	6	0
4	B	179	0	0	14	0
All	All	5008	0	4778	183	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 19.

All (183) 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:203:MET:HE1	1:A:243:PHE:HA	1.25	1.18
1:B:203:MET:HE1	1:B:243:PHE:HA	1.34	1.07
1:B:28:LEU:HD11	1:B:61:ARG:HB2	1.48	0.96
1:B:161:ILE:HD13	1:B:176:ALA:HA	1.47	0.95
1:A:234:GLN:NE2	1:A:234:GLN:H	1.67	0.92
1:B:8:LYS:HE2	1:B:303:GLU:HG3	1.56	0.88
1:B:29:GLU:CD	4:B:1067:HOH:O	2.12	0.87
1:B:29:GLU:HG3	4:B:1067:HOH:O	1.74	0.85
1:B:1:MET:HG2	1:B:2:GLY:H	1.45	0.82
1:B:29:GLU:CG	4:B:1067:HOH:O	2.27	0.81
1:A:65:LYS:NZ	1:A:303:GLU:OE2	2.14	0.81
1:A:299:GLU:OE2	1:A:303:GLU:HG3	1.84	0.77
1:B:115:LYS:HE2	4:B:958:HOH:O	1.84	0.77
1:A:36:GLU:CD	1:B:37:MET:HE2	2.05	0.76
1:B:201:ASN:HD22	1:B:204:GLU:HG2	1.52	0.74
1:A:55:GLU:HB3	1:A:71:LYS:NZ	2.03	0.73
1:A:36:GLU:CG	1:B:37:MET:HE2	2.19	0.72
1:A:44:VAL:O	1:A:268:PRO:HG3	1.90	0.71
1:A:211:ARG:HD3	3:A:908:EDO:H21	1.72	0.70
1:B:137:ALA:HB1	1:B:146:GLY:HA2	1.74	0.68
1:A:142:ARG:HE	1:A:195:ARG:NH2	1.92	0.68
1:B:161:ILE:CD1	1:B:176:ALA:HA	2.22	0.67
1:A:203:MET:HE3	1:A:246:ALA:HB3	1.76	0.67
1:A:37:MET:SD	1:B:36:GLU:OE1	2.53	0.67
1:A:203:MET:HE1	1:A:243:PHE:CA	2.16	0.66
1:B:29:GLU:OE2	4:B:1067:HOH:O	2.13	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:HD22	1:A:204:GLU:H	1.43	0.66
1:B:3:PHE:O	1:B:6:ARG:HG2	1.96	0.66
1:A:33:GLU:OE1	1:B:33:GLU:HG3	1.96	0.66
2:A:755:SO4:O4	1:B:195:ARG:HD3	1.96	0.65
1:A:265:VAL:O	1:A:268:PRO:HD2	1.97	0.65
1:A:142:ARG:HE	1:A:195:ARG:HH21	1.44	0.64
1:A:140:THR:HG22	4:A:914:HOH:O	1.98	0.64
1:B:16:GLU:HG3	1:B:17:ARG:N	2.14	0.63
1:A:234:GLN:H	1:A:234:GLN:HE21	1.47	0.62
1:A:16:GLU:OE1	1:A:20:LYS:HE2	1.99	0.62
1:B:55:GLU:HG2	1:B:71:LYS:HD3	1.82	0.62
1:B:232:THR:HG22	1:B:233:GLY:N	2.15	0.61
1:A:203:MET:HE3	1:A:246:ALA:CB	2.31	0.60
1:A:138:GLY:HA3	1:A:191:ASP:O	2.00	0.60
1:B:267:ILE:HB	1:B:268:PRO:HD3	1.83	0.60
1:B:265:VAL:O	1:B:268:PRO:HD2	2.02	0.60
1:A:46:LEU:HD22	1:A:50:GLU:HG3	1.84	0.60
1:A:142:ARG:HE	1:A:195:ARG:NE	2.00	0.60
1:A:43:ASP:OD2	1:A:234:GLN:NE2	2.35	0.60
1:A:30:GLU:O	1:A:34:GLU:HG2	2.02	0.59
1:B:201:ASN:ND2	1:B:204:GLU:HG2	2.17	0.59
1:A:234:GLN:HG3	1:B:262:LYS:HE3	1.84	0.59
1:A:267:ILE:HB	1:A:268:PRO:HD3	1.85	0.59
1:A:33:GLU:CD	1:B:33:GLU:HG3	2.23	0.58
3:A:900:EDO:H21	4:A:1074:HOH:O	2.03	0.58
1:B:23:PRO:HD3	1:B:34:GLU:OE1	2.03	0.58
1:A:203:MET:CE	1:A:246:ALA:HB3	2.32	0.58
1:B:8:LYS:CE	1:B:303:GLU:HG3	2.31	0.58
1:B:265:VAL:C	1:B:268:PRO:HD2	2.23	0.58
1:A:238:GLU:H	1:A:238:GLU:CD	2.05	0.58
1:B:211:ARG:HD3	4:B:1054:HOH:O	2.04	0.57
1:A:234:GLN:N	1:A:234:GLN:NE2	2.48	0.57
1:B:65:LYS:O	1:B:69:LYS:HG3	2.05	0.56
1:A:55:GLU:HB3	1:A:71:LYS:HZ3	1.70	0.56
1:B:3:PHE:CD1	1:B:95:PRO:HD3	2.40	0.56
1:A:142:ARG:HE	1:A:195:ARG:CZ	2.19	0.56
1:A:47:SER:OG	1:A:271:ARG:NH2	2.39	0.56
1:B:1:MET:CG	1:B:2:GLY:H	2.11	0.56
1:A:178:GLN:HE22	1:A:181:LYS:NZ	2.03	0.55
1:B:32:LEU:HD13	1:B:57:ARG:HE	1.71	0.55
1:A:37:MET:SD	1:B:36:GLU:CD	2.85	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG13	1:B:32:LEU:N	2.22	0.55
1:B:4:PHE:CE1	1:B:8:LYS:HE3	2.41	0.55
1:A:15:ARG:CD	1:A:304:ASP:OXT	2.55	0.55
1:B:258:ASP:OD2	1:B:283:GLY:HA2	2.06	0.55
1:A:220:GLU:O	3:A:907:EDO:H22	2.06	0.55
1:B:232:THR:HG22	1:B:233:GLY:H	1.72	0.55
1:A:143:ALA:O	1:A:144:ALA:C	2.45	0.54
1:A:142:ARG:HE	1:A:195:ARG:HE	1.54	0.54
1:B:48:ALA:HA	1:B:271:ARG:NH2	2.22	0.54
1:A:242:LYS:HD3	4:A:1118:HOH:O	2.07	0.54
1:A:147:THR:HG23	1:A:151:GLU:OE1	2.07	0.54
1:B:203:MET:CE	1:B:246:ALA:HB3	2.38	0.54
1:A:237:LEU:O	1:A:241:LYS:HG3	2.08	0.54
1:A:238:GLU:OE2	1:A:238:GLU:N	2.38	0.53
1:A:15:ARG:HD2	1:A:16:GLU:OE2	2.08	0.53
1:A:50:GLU:O	1:A:54:GLN:HG3	2.08	0.53
1:B:203:MET:HE3	1:B:246:ALA:HB3	1.90	0.53
1:B:31:VAL:HG21	1:B:64:LEU:HD11	1.91	0.52
1:A:4:PHE:CE2	1:A:8:LYS:HE3	2.45	0.52
1:A:211:ARG:HD3	3:A:908:EDO:C2	2.38	0.52
1:A:203:MET:CE	1:A:246:ALA:CB	2.87	0.52
1:A:15:ARG:NH1	1:A:304:ASP:OXT	2.42	0.52
1:B:102:GLY:HA3	1:B:222:LYS:HD2	1.92	0.51
1:A:132:LYS:HG2	1:A:185:TYR:CE2	2.45	0.51
1:B:211:ARG:CD	4:B:1054:HOH:O	2.58	0.51
1:B:13:LYS:O	1:B:16:GLU:HG2	2.11	0.51
1:B:28:LEU:CD1	1:B:61:ARG:HB2	2.30	0.51
1:A:199:LYS:HB3	1:A:199:LYS:NZ	2.27	0.50
1:A:142:ARG:NE	1:A:195:ARG:HE	2.09	0.50
1:B:139:ASP:OD2	1:B:142:ARG:HD3	2.11	0.50
1:A:229:ASP:OD1	1:A:231:VAL:HB	2.11	0.50
1:A:72:LEU:HD22	1:A:267:ILE:HD11	1.93	0.50
1:A:178:GLN:HE22	1:A:181:LYS:HZ3	1.60	0.49
1:A:55:GLU:CD	1:A:71:LYS:HD2	2.31	0.49
1:B:211:ARG:NH1	4:B:1054:HOH:O	2.16	0.49
1:B:229:ASP:OD1	1:B:231:VAL:HG23	2.12	0.49
1:A:111:ASN:HD21	1:A:142:ARG:CZ	2.25	0.49
1:A:132:LYS:HG2	1:A:185:TYR:CD2	2.46	0.49
1:A:17:ARG:HH12	3:A:901:EDO:H11	1.76	0.48
1:B:61:ARG:O	1:B:62:LYS:C	2.51	0.48
1:B:220:GLU:HB3	1:B:221:PRO:HA	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:PRO:HD2	4:B:980:HOH:O	2.14	0.48
1:B:102:GLY:CA	1:B:222:LYS:HD2	2.44	0.48
1:A:203:MET:HE2	1:A:242:LYS:O	2.14	0.48
1:A:65:LYS:CE	1:A:303:GLU:OE2	2.62	0.47
1:A:78:PRO:HG3	1:A:270:VAL:HG13	1.96	0.47
1:A:79:ASP:OD2	1:A:82:ARG:HG3	2.13	0.47
1:A:142:ARG:HH12	1:A:144:ALA:HA	1.80	0.47
1:A:234:GLN:N	1:A:234:GLN:HE21	2.09	0.47
1:B:28:LEU:HD11	1:B:61:ARG:CB	2.32	0.46
1:B:278:LYS:HZ3	3:B:903:EDO:H12	1.81	0.46
1:A:10:GLY:O	1:A:258:ASP:HA	2.16	0.46
1:B:44:VAL:O	1:B:268:PRO:HG3	2.16	0.46
1:B:75:MET:HB2	1:B:75:MET:HE3	1.59	0.46
1:B:28:LEU:O	1:B:29:GLU:HG3	2.16	0.46
1:A:142:ARG:CD	1:A:195:ARG:HE	2.29	0.46
1:A:242:LYS:HE3	4:A:1088:HOH:O	2.14	0.46
1:A:244:HIS:HA	1:A:249:LEU:HG	1.98	0.45
1:B:250:THR:HB	3:B:903:EDO:H22	1.98	0.45
1:B:181:LYS:HE2	1:B:217:ASP:OD1	2.16	0.45
1:A:55:GLU:HB3	1:A:71:LYS:HZ2	1.79	0.45
1:B:49:THR:O	1:B:53:LEU:HD23	2.17	0.45
1:B:278:LYS:HZ1	3:B:903:EDO:H21	1.81	0.45
1:B:69:LYS:HG2	1:B:302:LEU:HD12	1.99	0.45
3:B:904:EDO:C2	4:B:1080:HOH:O	2.64	0.45
1:A:52:ILE:HD13	1:A:72:LEU:HD21	1.99	0.45
1:B:10:GLY:O	1:B:258:ASP:HA	2.17	0.44
1:B:13:LYS:HG2	1:B:261:ALA:HB2	1.99	0.44
3:B:904:EDO:H22	4:B:1080:HOH:O	2.16	0.44
1:B:98:VAL:HG23	1:B:291:PRO:HB3	1.99	0.44
1:A:238:GLU:HG3	4:A:1078:HOH:O	2.15	0.44
1:A:220:GLU:HB3	1:A:221:PRO:HA	1.99	0.44
1:B:183:ARG:HD2	4:B:1039:HOH:O	2.17	0.44
1:B:201:ASN:HD22	1:B:204:GLU:H	1.65	0.44
1:B:3:PHE:CE1	1:B:95:PRO:HD3	2.52	0.44
1:B:203:MET:CE	1:B:246:ALA:CB	2.96	0.44
1:A:1:MET:O	1:A:6:ARG:CZ	2.66	0.44
1:B:134:MET:SD	1:B:161:ILE:HD11	2.58	0.44
1:B:233:GLY:O	1:B:236:GLY:N	2.51	0.43
1:A:142:ARG:HH21	1:A:195:ARG:NH2	2.16	0.43
1:A:64:LEU:O	1:A:68:VAL:HG23	2.18	0.43
1:B:201:ASN:HD21	1:B:203:MET:HB2	1.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HG22	1:A:236:GLY:H	1.83	0.43
1:A:302:LEU:N	1:A:302:LEU:HD12	2.32	0.43
1:A:101:LYS:HG2	1:A:222:LYS:HD3	2.00	0.43
1:A:254:VAL:HG21	1:A:266:LEU:HD22	2.01	0.43
1:B:64:LEU:O	1:B:68:VAL:HG23	2.18	0.43
1:A:265:VAL:C	1:A:268:PRO:HD2	2.38	0.43
1:A:36:GLU:CG	1:A:53:LEU:HD11	2.49	0.42
1:A:36:GLU:HB3	1:B:37:MET:HE2	2.01	0.42
1:B:16:GLU:HG3	1:B:17:ARG:H	1.84	0.42
1:A:142:ARG:NE	1:A:195:ARG:NE	2.65	0.42
1:A:301:LEU:HB3	1:A:302:LEU:HD12	2.00	0.42
1:B:145:GLY:HA2	4:B:1051:HOH:O	2.17	0.42
1:A:36:GLU:HG3	1:A:53:LEU:HD11	2.02	0.42
1:B:158:ILE:HA	1:B:159:PRO:HD3	1.84	0.42
1:A:23:PRO:O	1:A:25:GLY:N	2.53	0.42
1:B:238:GLU:OE2	1:B:238:GLU:HA	2.20	0.42
1:A:4:PHE:CZ	1:A:8:LYS:HE3	2.56	0.41
1:B:161:ILE:HD11	1:B:179:ALA:HB3	2.03	0.41
1:A:142:ARG:HD3	4:A:921:HOH:O	2.19	0.41
1:A:282:VAL:HG22	1:A:288:ASP:O	2.21	0.41
1:B:203:MET:HE3	1:B:246:ALA:CB	2.49	0.41
1:B:197:HIS:HE1	4:B:1033:HOH:O	2.02	0.41
1:B:1:MET:CG	1:B:2:GLY:N	2.80	0.41
1:B:237:LEU:O	1:B:241:LYS:HG3	2.20	0.41
1:A:36:GLU:CB	1:B:37:MET:HE2	2.50	0.41
1:A:234:GLN:O	1:A:238:GLU:OE2	2.38	0.41
1:B:139:ASP:OD1	1:B:193:ALA:HA	2.20	0.41
1:A:254:VAL:HG11	1:A:266:LEU:HD21	2.02	0.41
1:A:98:VAL:HG23	1:A:291:PRO:HB3	2.03	0.41
1:B:97:PRO:HA	1:B:125:TYR:OH	2.21	0.41
1:A:303:GLU:O	1:A:304:ASP:HB2	2.21	0.40
1:B:232:THR:CG2	1:B:233:GLY:N	2.84	0.40
1:B:64:LEU:HD23	1:B:64:LEU:H	1.86	0.40
1:B:72:LEU:HD12	1:B:302:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	302/304 (99%)	285 (94%)	14 (5%)	3 (1%)	18	14
1	B	286/304 (94%)	275 (96%)	8 (3%)	3 (1%)	18	14
All	All	588/608 (97%)	560 (95%)	22 (4%)	6 (1%)	18	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	LYS
1	A	57	ARG
1	A	144	ALA
1	A	24	TRP
1	B	59	SER
1	B	248	GLY

### 5.3.2 Protein sidechains

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	242/242 (100%)	232 (96%)	10 (4%)	35	39
1	B	230/242 (95%)	227 (99%)	3 (1%)	73	82
All	All	472/484 (98%)	459 (97%)	13 (3%)	49	57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	27	ASN
1	A	35	LEU
1	A	43	ASP
1	A	46	LEU
1	A	81	ARG
1	A	199	LYS
1	A	234	GLN
1	A	238	GLU
1	A	304	ASP
1	B	3	PHE
1	B	27	ASN
1	B	54	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	54	GLN
1	A	91	ASN
1	A	93	GLN
1	A	111	ASN
1	A	148	GLN
1	A	178	GLN
1	A	201	ASN
1	A	234	GLN
1	A	239	GLN
1	B	54	GLN
1	B	111	ASN
1	B	162	GLN
1	B	201	ASN
1	B	234	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	SO4	A	750	-	4,4,4	0.32	0	6,6,6	0.44	0
2	SO4	A	752	-	4,4,4	0.37	0	6,6,6	0.86	0
2	SO4	A	753	-	4,4,4	0.41	0	6,6,6	0.73	0
2	SO4	A	755	-	4,4,4	0.39	0	6,6,6	0.71	0
2	SO4	A	757	-	4,4,4	0.35	0	6,6,6	0.50	0
3	EDO	A	900	-	3,3,3	0.43	0	2,2,2	0.45	0
3	EDO	A	901	-	3,3,3	0.54	0	2,2,2	0.52	0
3	EDO	A	905	-	3,3,3	0.43	0	2,2,2	0.06	0
3	EDO	A	906	-	3,3,3	0.36	0	2,2,2	0.63	0
3	EDO	A	907	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	A	908	-	3,3,3	0.14	0	2,2,2	0.75	0
2	SO4	B	751	-	4,4,4	0.30	0	6,6,6	0.59	0
2	SO4	B	756	-	4,4,4	0.23	0	6,6,6	0.81	0
2	SO4	B	758	-	4,4,4	0.42	0	6,6,6	0.25	0
2	SO4	B	759	-	4,4,4	0.28	0	6,6,6	0.62	0
3	EDO	B	902	-	3,3,3	0.34	0	2,2,2	0.14	0
3	EDO	B	903	-	3,3,3	0.40	0	2,2,2	0.46	0
3	EDO	B	904	-	3,3,3	0.57	0	2,2,2	0.53	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	SO4	A	750	-	-	0/0/0/0	0/0/0/0
2	SO4	A	752	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	753	-	-	0/0/0/0	0/0/0/0
2	SO4	A	755	-	-	0/0/0/0	0/0/0/0
2	SO4	A	757	-	-	0/0/0/0	0/0/0/0
3	EDO	A	900	-	-	0/1/1/1	0/0/0/0
3	EDO	A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	A	905	-	-	0/1/1/1	0/0/0/0
3	EDO	A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	A	908	-	-	0/1/1/1	0/0/0/0
2	SO4	B	751	-	-	0/0/0/0	0/0/0/0
2	SO4	B	756	-	-	0/0/0/0	0/0/0/0
2	SO4	B	758	-	-	0/0/0/0	0/0/0/0
2	SO4	B	759	-	-	0/0/0/0	0/0/0/0
3	EDO	B	902	-	-	0/1/1/1	0/0/0/0
3	EDO	B	903	-	-	0/1/1/1	0/0/0/0
3	EDO	B	904	-	-	0/1/1/1	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.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	755	SO4	1	0
3	A	900	EDO	1	0
3	A	901	EDO	1	0
3	A	907	EDO	1	0
3	A	908	EDO	2	0
3	B	903	EDO	3	0
3	B	904	EDO	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	304/304 (100%)	0.92	38 (12%) <b>4</b> <b>4</b>	20, 26, 35, 42	0
1	B	290/304 (95%)	1.08	52 (17%) <b>2</b> <b>1</b>	20, 26, 33, 40	0
All	All	594/608 (97%)	1.00	90 (15%) <b>2</b> <b>2</b>	20, 26, 34, 42	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	GLY	11.0
1	A	143	ALA	10.0
1	A	144	ALA	9.0
1	A	145	GLY	7.1
1	A	304	ASP	6.9
1	A	58	ALA	6.9
1	B	1	MET	6.9
1	B	58	ALA	6.9
1	B	60	GLY	6.8
1	B	61	ARG	6.6
1	B	234	GLN	6.3
1	B	25	GLY	5.8
1	B	97	PRO	5.8
1	A	1	MET	5.6
1	A	141	PHE	5.5
1	B	29	GLU	5.3
1	B	147	THR	5.3
1	A	60	GLY	5.2
1	B	144	ALA	5.2
1	B	304	ASP	5.1
1	B	235	ASN	5.0
1	B	79	ASP	4.9
1	B	63	ASP	4.8
1	A	59	SER	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	93	GLN	4.6
1	B	96	LYS	4.4
1	B	145	GLY	4.4
1	A	29	GLU	4.2
1	A	57	ARG	4.1
1	A	2	GLY	4.0
1	B	62	LYS	4.0
1	B	24	TRP	3.9
1	A	90	PHE	3.8
1	A	91	ASN	3.8
1	A	61	ARG	3.7
1	A	140	THR	3.7
1	B	95	PRO	3.6
1	B	2	GLY	3.6
1	A	94	LYS	3.5
1	B	3	PHE	3.5
1	B	233	GLY	3.4
1	A	95	PRO	3.3
1	A	146	GLY	3.3
1	A	238	GLU	3.2
1	B	200	HIS	3.1
1	A	92	PRO	3.1
1	B	27	ASN	3.1
1	B	106	LEU	3.1
1	B	30	GLU	3.1
1	B	28	LEU	3.0
1	B	236	GLY	3.0
1	A	190	VAL	3.0
1	B	143	ALA	2.9
1	A	62	LYS	2.9
1	A	28	LEU	2.8
1	B	190	VAL	2.8
1	A	235	ASN	2.8
1	B	31	VAL	2.7
1	A	25	GLY	2.7
1	B	166	GLY	2.7
1	B	23	PRO	2.7
1	B	22	ILE	2.7
1	B	4	PHE	2.7
1	A	142	ARG	2.6
1	B	54	GLN	2.5
1	B	55	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	199	LYS	2.5
1	A	237	LEU	2.5
1	B	6	ARG	2.5
1	B	245	GLU	2.5
1	A	27	ASN	2.5
1	B	59	SER	2.4
1	B	108	VAL	2.3
1	A	107	VAL	2.2
1	B	165	GLU	2.2
1	B	224	VAL	2.2
1	A	119	ILE	2.2
1	A	188	LEU	2.2
1	B	177	VAL	2.2
1	A	105	VAL	2.1
1	B	77	GLU	2.1
1	A	286	PRO	2.1
1	A	209	VAL	2.1
1	A	302	LEU	2.1
1	B	98	VAL	2.1
1	B	252	VAL	2.1
1	A	30	GLU	2.1
1	B	280	VAL	2.1
1	B	101	LYS	2.0
1	B	135	PHE	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
3	EDO	A	901	4/4	0.87	0.37	16.50	33,39,40,47	0
3	EDO	B	904	4/4	0.80	0.48	8.30	43,50,53,58	0
3	EDO	A	908	4/4	0.71	0.45	5.27	59,59,61,64	0
3	EDO	B	903	4/4	0.76	0.41	4.12	48,52,53,54	0
3	EDO	A	906	4/4	0.77	0.29	3.30	61,63,65,66	0
2	SO4	A	752	5/5	0.69	0.30	2.44	49,55,60,62	0
3	EDO	A	900	4/4	0.50	0.43	1.98	59,60,63,64	0
2	SO4	A	757	5/5	0.94	0.20	0.91	64,65,68,69	0
3	EDO	A	907	4/4	0.80	0.21	0.87	52,58,58,59	0
2	SO4	A	750	5/5	0.99	0.17	0.44	42,46,49,50	0
2	SO4	B	751	5/5	0.97	0.14	0.12	41,42,49,50	0
2	SO4	A	755	5/5	0.98	0.15	-0.08	43,44,48,49	0
2	SO4	A	753	5/5	0.93	0.18	-0.46	47,50,55,57	0
2	SO4	B	759	5/5	0.91	0.20	-	59,60,64,64	0
3	EDO	B	902	4/4	0.72	0.31	-	59,61,63,65	0
2	SO4	B	756	5/5	0.93	0.19	-	47,53,58,60	0
3	EDO	A	905	4/4	0.72	0.55	-	63,65,65,66	0
2	SO4	B	758	5/5	0.88	0.18	-	60,60,62,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.