



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 AM GMT

PDB ID : 3EO4  
Title : The crystal structure of a domain from Methanocaldococcus jannaschii DSM 2661  
Authors : Tan, K.; Hatzos, C.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-09-26  
Resolution : 2.19 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

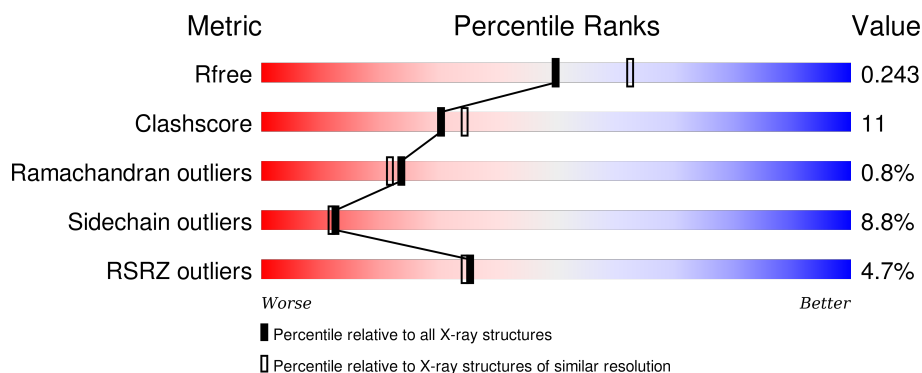
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	164	<div> <div>4%</div> <div>73%</div> <div>16%</div> <div>6%</div> <div>• •</div> </div>
1	B	164	<div> <div>77%</div> <div>12%</div> <div>•</div> <div>7%</div> </div>
1	C	164	<div> <div>6%</div> <div>66%</div> <div>22%</div> <div>5%</div> <div>6%</div> </div>
1	D	164	<div> <div>8%</div> <div>73%</div> <div>23%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MES	A	8	-	-	-	X
2	MES	B	5	-	-	-	X
2	MES	C	6	-	-	-	X
2	MES	D	7	-	-	-	X
4	EDO	D	2	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5710 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.

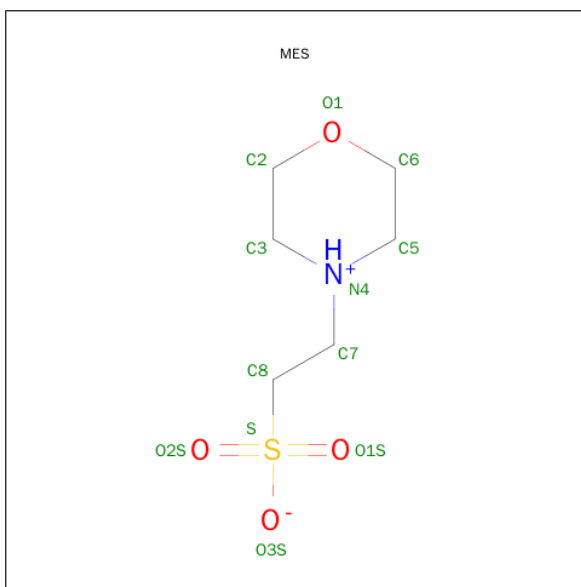
- Molecule 1 is a protein called Uncharacterized protein MJ1062.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	Se	0	1	0
			1347	875	238	231	1	2			
1	B	152	Total	C	N	O	Se		0	3	0
			1319	860	232	225	2				
1	C	154	Total	C	N	O	Se		0	0	0
			1313	854	231	226	2				
1	D	162	Total	C	N	O	S	Se	0	0	0
			1371	889	242	237	1	2			

There are 12 discrepancies between the modelled and reference sequences:

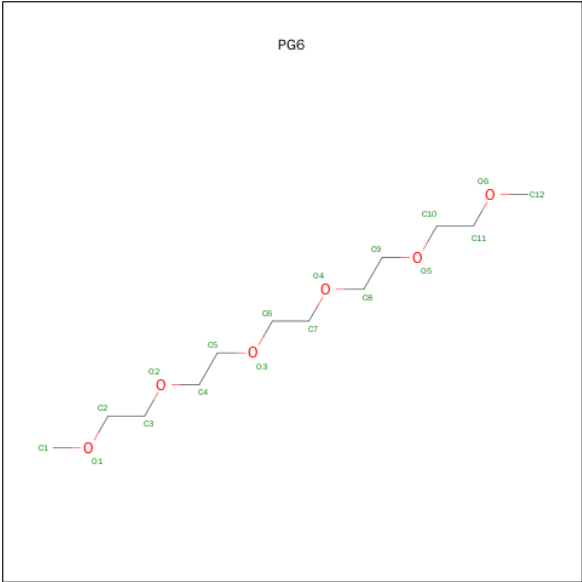
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	SER	-	expression tag	UNP Q58462
A	340	ASN	-	expression tag	UNP Q58462
A	341	ALA	-	expression tag	UNP Q58462
B	339	SER	-	expression tag	UNP Q58462
B	340	ASN	-	expression tag	UNP Q58462
B	341	ALA	-	expression tag	UNP Q58462
C	339	SER	-	expression tag	UNP Q58462
C	340	ASN	-	expression tag	UNP Q58462
C	341	ALA	-	expression tag	UNP Q58462
D	339	SER	-	expression tag	UNP Q58462
D	340	ASN	-	expression tag	UNP Q58462
D	341	ALA	-	expression tag	UNP Q58462

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



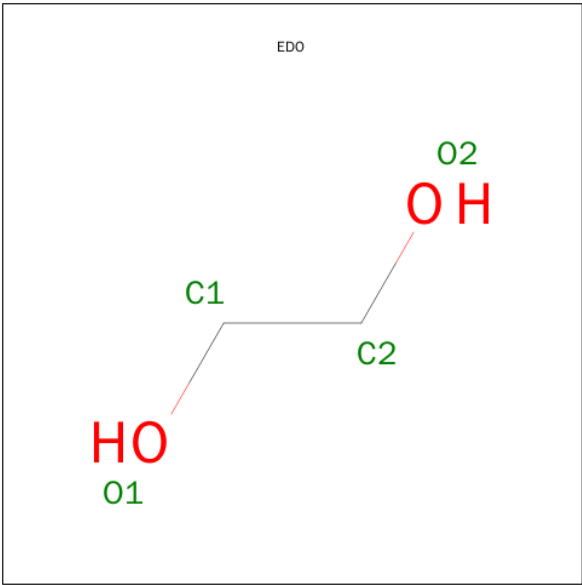
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 4 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
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total 68	O 68	0	0
5	B	50	Total 50	O 50	0	0
5	C	58	Total 58	O 58	0	0
5	D	58	Total 58	O 58	0	0



- Molecule 1: Uncharacterized protein MJ1062





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.37Å 96.87Å 83.21Å 90.00° 126.63° 90.00°	Depositor
Resolution (Å)	48.45 – 2.19 48.44 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.45-2.19) 97.5 (48.44-2.19)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, $R_{free}$	0.195 , 0.240 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	2072 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41222 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: PG6, EDO, MES

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	0.67	0/1380	0.77	1/1853 (0.1%)
1	B	0.69	0/1359	0.74	0/1827
1	C	0.59	0/1344	0.73	1/1808 (0.1%)
1	D	0.58	0/1402	0.72	0/1884
All	All	0.63	0/5485	0.74	2/7372 (0.0%)

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
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	385	LEU	CA-CB-CG	5.29	127.45	115.30
1	A	434	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	358	THR	Peptide

## 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	1347	0	1376	29	0
1	B	1319	0	1351	20	0
1	C	1313	0	1335	41	0
1	D	1371	0	1397	31	0
2	A	24	0	24	5	0
2	B	24	0	24	3	0
2	C	24	0	24	8	0
2	D	24	0	24	4	0
3	A	18	0	26	1	0
4	B	4	0	6	0	0
4	C	4	0	6	1	0
4	D	4	0	6	7	0
5	A	68	0	0	3	0
5	B	50	0	0	1	0
5	C	58	0	0	3	0
5	D	58	0	0	1	0
All	All	5710	0	5599	122	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 11.

All (122) 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:D:367:ALA:HA	4:D:2:EDO:H21	1.23	1.10
1:A:474:ILE:HD11	1:A:478:LYS:HE3	1.29	1.10
1:C:436:GLY:O	4:D:2:EDO:H12	1.66	0.96
1:D:367:ALA:HA	4:D:2:EDO:C2	1.96	0.95
1:A:406:LEU:HG	1:A:413:ILE:CD1	1.96	0.95
1:A:406:LEU:HG	1:A:413:ILE:HD13	1.51	0.90
1:D:367:ALA:CA	4:D:2:EDO:H21	2.04	0.88
1:A:425:ASN:HD22	1:A:425:ASN:H	1.20	0.88
1:D:370:SER:HB2	4:D:2:EDO:H22	1.69	0.73
1:B:435:ILE:HD11	1:B:440:LEU:HB2	1.73	0.71
1:C:432:GLY:HA2	2:C:6:MES:H32	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ARG:HG2	1:D:413:ILE:HG12	1.74	0.70
1:B:472:ASN:H	1:B:472:ASN:HD22	1.40	0.69
1:A:432:GLY:CA	2:A:8:MES:H71	2.22	0.69
1:D:344:LYS:HB3	1:D:448:HIS:CE1	2.29	0.68
1:C:436:GLY:O	4:D:2:EDO:C1	2.40	0.67
1:A:358:THR:HG22	1:A:360:ASN:H	1.59	0.67
1:C:357:ILE:HD11	1:C:394:TRP:HZ3	1.59	0.67
1:D:344:LYS:HB3	1:D:448:HIS:NE2	2.11	0.65
1:A:406:LEU:CG	1:A:413:ILE:HD13	2.26	0.65
1:C:427:ASP:OD1	1:C:427:ASP:N	2.30	0.65
1:D:476:SER:HB2	2:D:3:MES:H61	1.78	0.65
1:B:421:VAL:HG11	1:B:457:LEU:HD11	1.79	0.64
1:B:382:LYS:HD3	1:C:376:LYS:O	1.97	0.64
1:C:357:ILE:CD1	1:C:394:TRP:HZ3	2.10	0.63
1:C:435:ILE:HD13	2:C:4:MES:H82	1.80	0.63
1:D:357:ILE:HD12	1:D:402:ASP:HB2	1.81	0.62
1:C:408:ARG:HG3	1:C:413:ILE:HG22	1.82	0.61
1:D:475:ARG:HD2	5:D:39:HOH:O	2.00	0.61
1:A:425:ASN:ND2	1:A:425:ASN:H	1.96	0.61
1:D:492:ARG:H	1:D:495:GLU:HB3	1.68	0.59
1:C:490:LYS:HG2	5:C:141:HOH:O	2.03	0.59
1:A:432:GLY:HA2	2:A:8:MES:H71	1.84	0.59
1:C:437:GLU:HB3	1:C:440:LEU:HD12	1.86	0.57
1:A:488:THR:HG22	1:A:489:LYS:HB2	1.84	0.57
1:B:388[B]:GLU:H	1:B:388[B]:GLU:CD	2.07	0.56
1:A:425:ASN:N	1:A:425:ASN:HD22	1.92	0.56
1:B:432:GLY:HA2	2:B:5:MES:H51	1.88	0.56
1:A:421:VAL:HG12	1:A:431:ILE:CD1	2.36	0.56
3:A:1:PG6:H32	5:A:187:HOH:O	2.06	0.55
1:D:342:ASN:HB2	1:D:354:ILE:CG1	2.37	0.55
1:C:384:PRO:O	1:D:439:PHE:HE2	1.90	0.55
2:A:2:MES:H52	5:A:176:HOH:O	2.06	0.54
1:B:378:PHE:O	1:C:382:LYS:NZ	2.41	0.54
1:C:355:ARG:HH21	1:C:415:LYS:HZ2	1.56	0.54
1:A:343:CYS:HB2	1:A:452:LEU:HD11	1.90	0.53
1:C:433:ILE:H	2:C:6:MES:H31	1.74	0.53
1:D:386:LYS:HB2	1:D:389:GLU:HG3	1.92	0.52
1:D:370:SER:CB	4:D:2:EDO:H22	2.37	0.52
1:C:432:GLY:HA2	2:C:6:MES:C3	2.39	0.51
1:A:421:VAL:CG1	1:A:453:VAL:HG11	2.41	0.51
1:B:432:GLY:HA2	2:B:5:MES:C5	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:NH2	1:C:415:LYS:NZ	2.59	0.51
1:C:357:ILE:CD1	1:C:394:TRP:CZ3	2.94	0.50
1:B:376:LYS:O	1:C:382:LYS:HD3	2.11	0.50
1:A:421:VAL:HG12	1:A:431:ILE:HD13	1.93	0.50
1:D:421:VAL:HG12	1:D:431:ILE:HG12	1.93	0.50
1:D:492:ARG:N	1:D:495:GLU:HB3	2.26	0.49
1:D:479:LEU:HD23	1:D:479:LEU:C	2.33	0.49
1:C:479:LEU:C	1:C:479:LEU:HD23	2.34	0.48
1:A:373:LEU:HB3	1:A:438:PHE:HE1	1.78	0.48
1:A:358:THR:HG22	1:A:360:ASN:N	2.26	0.48
1:A:359[A]:ASP:OD1	1:A:394:TRP:CZ2	2.66	0.48
1:C:415:LYS:HE2	5:C:94:HOH:O	2.13	0.48
1:A:404:ILE:HG21	1:A:415:LYS:HG2	1.95	0.48
1:D:468:ARG:HB3	1:D:497:ILE:HD13	1.95	0.47
1:C:421:VAL:HG13	1:C:453:VAL:HG11	1.95	0.47
1:C:433:ILE:O	2:C:6:MES:H51	2.14	0.47
1:C:476:SER:HB2	2:C:4:MES:H61	1.95	0.47
1:C:355:ARG:HH21	1:C:415:LYS:NZ	2.13	0.46
1:C:468:ARG:HG2	1:C:497:ILE:HD13	1.97	0.46
1:B:421:VAL:HG13	1:B:431:ILE:HG12	1.97	0.46
1:A:421:VAL:CG1	1:A:453:VAL:CG1	2.93	0.46
1:D:408:ARG:CG	1:D:413:ILE:HG12	2.45	0.46
1:D:346:ILE:HG21	1:D:352:ILE:HD12	1.97	0.46
1:C:388:GLU:O	1:C:392:SER:HB2	2.16	0.46
1:C:393:TRP:O	1:C:397:ARG:HG3	2.14	0.46
1:B:408:ARG:NH2	1:B:408:ARG:HB2	2.31	0.45
1:B:386:LYS:HB3	1:B:388[B]:GLU:OE1	2.16	0.45
1:B:408:ARG:CB	1:B:408:ARG:HH21	2.30	0.45
1:B:490:LYS:HD3	5:B:189:HOH:O	2.16	0.45
1:C:444:HIS:HA	5:C:195:HOH:O	2.17	0.45
1:B:362:LEU:HD21	1:B:394:TRP:CD2	2.52	0.45
1:C:477:ILE:O	1:C:481:GLU:HG3	2.17	0.45
1:A:358:THR:CG2	1:A:360:ASN:H	2.29	0.44
2:D:3:MES:H52	2:D:3:MES:H81	1.62	0.44
1:C:421:VAL:HG21	1:C:456:TRP:CZ3	2.52	0.44
1:C:388:GLU:H	1:C:388:GLU:CD	2.20	0.44
1:C:479:LEU:O	1:C:479:LEU:HD23	2.17	0.44
1:A:382:LYS:HD3	1:D:376:LYS:O	2.16	0.44
1:C:390:HIS:HD1	4:C:3:EDO:HO1	1.60	0.44
1:D:364:LEU:HD13	1:D:368:TRP:CH2	2.53	0.44
2:A:2:MES:H22	5:A:176:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:CYS:N	1:A:352:ILE:O	2.51	0.43
1:D:368:TRP:HB3	1:D:434:LEU:HD21	1.99	0.43
1:A:368:TRP:HB3	1:A:434:LEU:HD21	2.00	0.43
1:C:373:LEU:HB3	1:C:438:PHE:CE1	2.53	0.43
1:D:430:GLU:HB2	1:D:466:HIS:CE1	2.54	0.43
1:D:388:GLU:H	1:D:388:GLU:CD	2.22	0.43
1:D:432:GLY:HA2	2:D:7:MES:H32	2.00	0.43
1:C:421:VAL:HG21	1:C:456:TRP:HZ3	1.84	0.42
1:C:349:ASP:O	1:C:409:GLU:HA	2.20	0.42
1:D:471:GLU:HG3	1:D:496:TRP:CD1	2.55	0.42
1:A:379:TYR:CD2	1:A:380:ILE:HD13	2.55	0.42
1:A:425:ASN:N	1:A:425:ASN:ND2	2.62	0.42
1:C:435:ILE:HD11	1:C:446:GLY:HA2	2.02	0.41
1:D:357:ILE:CD1	1:D:402:ASP:HB2	2.48	0.41
1:A:343:CYS:SG	1:A:448:HIS:HB3	2.60	0.41
1:C:473:ASN:OD1	2:C:4:MES:H22	2.20	0.41
2:C:4:MES:H81	2:C:4:MES:H52	1.55	0.41
1:B:388[A]:GLU:HG3	1:B:388[A]:GLU:H	1.75	0.41
1:C:379:TYR:CE2	1:C:380:ILE:HD13	2.55	0.41
1:C:395:MSE:HB2	1:C:395:MSE:HE3	1.95	0.41
1:B:362:LEU:HD21	1:B:394:TRP:CE3	2.56	0.41
1:A:433:ILE:H	2:A:8:MES:H71	1.85	0.41
1:B:408:ARG:HB2	1:B:408:ARG:HH21	1.85	0.41
1:B:414:ARG:HG3	1:B:416:VAL:HG23	2.03	0.40
1:A:370:SER:HB3	1:A:384:PRO:HB3	2.02	0.40
1:B:366:MSE:HB2	1:B:390:HIS:CD2	2.56	0.40
2:B:1:MES:H32	2:B:1:MES:H81	1.54	0.40
1:D:342:ASN:HB2	1:D:354:ILE:HG12	2.02	0.40
1:D:432:GLY:HA2	2:D:7:MES:C3	2.52	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	155/164 (94%)	153 (99%)	1 (1%)	1 (1%)	30	29
1	B	153/164 (93%)	150 (98%)	2 (1%)	1 (1%)	26	25
1	C	152/164 (93%)	147 (97%)	4 (3%)	1 (1%)	26	25
1	D	160/164 (98%)	153 (96%)	5 (3%)	2 (1%)	15	11
All	All	620/656 (94%)	603 (97%)	12 (2%)	5 (1%)	24	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	ILE
1	C	359	ASP
1	A	380	ILE
1	D	380	ILE
1	D	346	ILE

### 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	147/149 (99%)	127 (86%)	20 (14%)	5	3
1	B	144/149 (97%)	133 (92%)	11 (8%)	16	16
1	C	143/149 (96%)	133 (93%)	10 (7%)	19	19
1	D	149/149 (100%)	138 (93%)	11 (7%)	17	17
All	All	583/596 (98%)	531 (91%)	52 (9%)	12	11

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	ASN
1	A	358	THR
1	A	373	LEU
1	A	380	ILE
1	A	382	LYS
1	A	385	LEU

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Mol	Chain	Res	Type
1	A	388	GLU
1	A	396	SER
1	A	398	GLU
1	A	406	LEU
1	A	413	ILE
1	A	415	LYS
1	A	425	ASN
1	A	433	ILE
1	A	434	LEU
1	A	464	LYS
1	A	474	ILE
1	A	488	THR
1	A	490	LYS
1	A	502	LEU
1	B	385	LEU
1	B	388[A]	GLU
1	B	388[B]	GLU
1	B	408	ARG
1	B	409	GLU
1	B	421	VAL
1	B	435	ILE
1	B	472	ASN
1	B	474	ILE
1	B	476	SER
1	B	490	LYS
1	C	349	ASP
1	C	359	ASP
1	C	373	LEU
1	C	382	LYS
1	C	385	LEU
1	C	388	GLU
1	C	392	SER
1	C	415	LYS
1	C	427	ASP
1	C	457	LEU
1	D	349	ASP
1	D	357	ILE
1	D	364	LEU
1	D	373	LEU
1	D	375	TYR
1	D	385	LEU
1	D	408	ARG

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Mol	Chain	Res	Type
1	D	410	ASN
1	D	455	LYS
1	D	471	GLU
1	D	501	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	GLN
1	A	411	ASN
1	A	425	ASN
1	A	494	ASN
1	B	423	GLN
1	B	472	ASN
1	B	494	ASN
1	C	423	GLN
1	C	494	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	PG6	A	1	-	17,17,17	0.60	0	16,16,16	0.77	1 (6%)
2	MES	A	2	-	11,12,12	0.67	0	14,16,16	3.17	5 (35%)
2	MES	A	8	-	11,12,12	0.73	0	14,16,16	2.46	3 (21%)
2	MES	B	1	-	11,12,12	0.56	0	14,16,16	2.99	5 (35%)
2	MES	B	5	-	11,12,12	0.69	0	14,16,16	2.61	6 (42%)
4	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	C	3	-	3,3,3	0.56	0	2,2,2	0.41	0
2	MES	C	4	-	11,12,12	0.77	0	14,16,16	2.54	5 (35%)
2	MES	C	6	-	11,12,12	0.77	0	14,16,16	2.32	4 (28%)
4	EDO	D	2	-	3,3,3	0.25	0	2,2,2	0.46	0
2	MES	D	3	-	11,12,12	0.67	0	14,16,16	2.53	6 (42%)
2	MES	D	7	-	11,12,12	0.72	0	14,16,16	2.51	5 (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
3	PG6	A	1	-	-	0/15/15/15	0/0/0/0
2	MES	A	2	-	-	0/6/14/14	0/1/1/1
2	MES	A	8	-	-	0/6/14/14	0/1/1/1
2	MES	B	1	-	-	0/6/14/14	0/1/1/1
2	MES	B	5	-	-	0/6/14/14	0/1/1/1
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	C	3	-	-	0/1/1/1	0/0/0/0
2	MES	C	4	-	-	0/6/14/14	0/1/1/1
2	MES	C	6	-	-	0/6/14/14	0/1/1/1
4	EDO	D	2	-	-	0/1/1/1	0/0/0/0
2	MES	D	3	-	-	0/6/14/14	0/1/1/1
2	MES	D	7	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MES	C6-C5-N4	-3.38	105.00	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	MES	C6-C5-N4	-3.26	105.19	110.12
2	B	1	MES	O3S-S-O1S	-2.80	105.08	111.61
2	B	5	MES	C2-C3-N4	-2.61	106.17	110.12
2	C	4	MES	O2S-S-O1S	-2.14	105.67	113.48
2	A	2	MES	C6-O1-C2	2.02	116.70	109.89
2	C	4	MES	O2S-S-C8	2.09	108.69	106.91
2	B	5	MES	O2S-S-C8	2.11	108.71	106.91
2	B	1	MES	C7-N4-C5	2.18	116.86	111.27
3	A	1	PG6	C10-O5-C9	2.29	123.13	113.31
2	D	3	MES	C7-N4-C3	2.62	117.99	111.27
2	D	7	MES	C7-N4-C3	2.66	118.08	111.27
2	D	7	MES	O2S-S-C8	2.81	109.31	106.91
2	D	3	MES	O1S-S-C8	2.88	109.36	106.91
2	A	2	MES	C7-N4-C5	2.88	118.66	111.27
2	C	6	MES	C7-N4-C3	2.90	118.70	111.27
2	B	5	MES	C7-N4-C5	2.96	118.87	111.27
2	D	3	MES	O2S-S-C8	3.01	109.48	106.91
2	B	5	MES	C7-N4-C3	3.05	119.09	111.27
2	C	4	MES	C7-N4-C5	3.16	119.37	111.27
2	C	4	MES	O1S-S-C8	3.21	109.64	106.91
2	C	6	MES	C7-N4-C5	3.27	119.66	111.27
2	A	2	MES	C7-N4-C3	3.44	120.08	111.27
2	A	8	MES	O2S-S-C8	3.66	110.03	106.91
2	D	7	MES	C7-N4-C5	3.74	120.86	111.27
2	D	3	MES	C7-N4-C5	3.86	121.17	111.27
2	A	8	MES	C7-N4-C3	3.97	121.45	111.27
2	B	1	MES	C7-N4-C3	3.99	121.50	111.27
2	D	7	MES	O1S-S-C8	4.13	110.43	106.91
2	B	5	MES	O1S-S-C8	4.51	110.75	106.91
2	D	3	MES	C5-N4-C3	5.50	120.82	108.90
2	D	7	MES	C5-N4-C3	5.62	121.06	108.90
2	A	2	MES	C5-N4-C3	5.70	121.24	108.90
2	B	1	MES	C5-N4-C3	5.87	121.62	108.90
2	C	6	MES	C5-N4-C3	5.88	121.63	108.90
2	B	5	MES	C5-N4-C3	6.07	122.05	108.90
2	A	8	MES	C5-N4-C3	6.24	122.42	108.90
2	B	1	MES	O2S-S-C8	6.88	112.77	106.91
2	C	4	MES	C5-N4-C3	7.19	124.46	108.90
2	A	2	MES	O2S-S-C8	8.44	114.11	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PG6	1	0
2	A	2	MES	2	0
2	A	8	MES	3	0
2	B	1	MES	1	0
2	B	5	MES	2	0
4	C	3	EDO	1	0
2	C	4	MES	4	0
2	C	6	MES	4	0
4	D	2	EDO	7	0
2	D	3	MES	2	0
2	D	7	MES	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	156/164 (95%)	0.38	6 (3%) 44 43	12, 19, 32, 62	0
1	B	150/164 (91%)	0.16	0 100 100	13, 20, 26, 31	0
1	C	152/164 (92%)	0.40	10 (6%) 22 21	16, 23, 31, 36	0
1	D	160/164 (97%)	0.59	13 (8%) 15 14	16, 23, 48, 62	0
All	All	618/656 (94%)	0.39	29 (4%) 35 34	12, 21, 31, 62	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	ALA	9.8
1	D	343	CYS	7.6
1	D	346	ILE	7.5
1	A	343	CYS	6.7
1	D	349	ASP	5.5
1	A	350	SER	5.4
1	D	342	ASN	5.1
1	D	347	GLY	4.2
1	D	502	LEU	4.2
1	D	345	LYS	4.1
1	C	350	SER	4.0
1	D	350	SER	3.9
1	A	341	ALA	3.8
1	C	502	LEU	3.6
1	D	348	GLU	3.5
1	A	345	LYS	3.3
1	C	353	ILE	3.2
1	C	460	ILE	3.2
1	A	342	ASN	3.1
1	A	344	LYS	3.1
1	D	344	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	459	ASN	2.4
1	C	349	ASP	2.4
1	D	460	ILE	2.4
1	D	457	LEU	2.4
1	C	455	LYS	2.3
1	C	461	GLY	2.2
1	C	427	ASP	2.0
1	C	463	LYS	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(Å <sup>2</sup> )	Q<0.9
2	MES	D	7	12/12	0.86	0.26	7.96	76,77,82,82	0
2	MES	C	6	12/12	0.83	0.21	3.75	65,67,76,76	0
2	MES	A	8	12/12	0.85	0.20	2.87	68,70,77,78	0
2	MES	B	5	12/12	0.86	0.19	2.40	70,71,76,76	0
3	PG6	A	1	18/18	0.90	0.15	1.31	39,46,51,52	0
4	EDO	D	2	4/4	0.95	0.17	1.30	30,30,31,35	0
2	MES	D	3	12/12	0.95	0.13	-0.07	48,50,55,56	0
2	MES	B	1	12/12	0.96	0.13	-0.14	46,47,50,51	0
2	MES	C	4	12/12	0.93	0.14	-0.26	46,49,52,52	0
2	MES	A	2	12/12	0.95	0.13	-0.73	45,47,50,50	0
4	EDO	B	503	4/4	0.89	0.11	-	49,50,50,52	0
4	EDO	C	3	4/4	0.80	0.14	-	41,47,47,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.