



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2016 – 05:44 PM EDT

PDB ID : 5IOB
Title : Crystal structure of beta-N-acetylglucosaminidase-like protein from *Corynebacterium glutamicum*
Authors : Chang, C.; Mack, J.; Endres, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2016-03-08
Resolution : 2.25 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

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

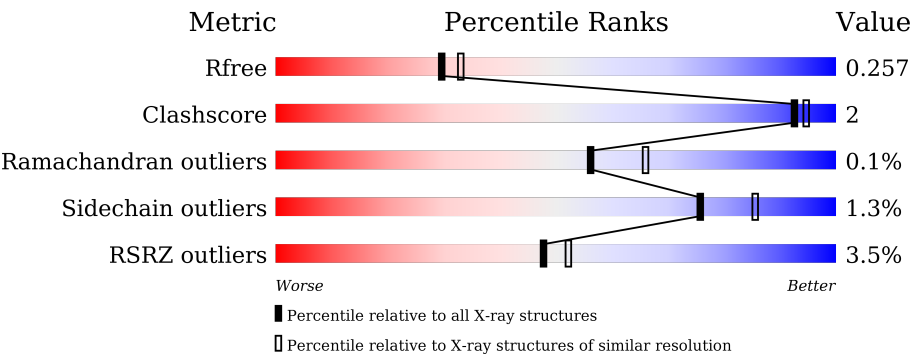
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 ≥ 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	348	<div><div>4%</div><div><div></div><div>86%</div><div>• •</div><div>9%</div></div></div>
1	B	348	<div><div>3%</div><div><div></div><div>87%</div><div>•</div><div>10%</div></div></div>
1	C	348	<div><div>2%</div><div><div></div><div>89%</div><div>•</div><div>8%</div></div></div>
1	D	348	<div><div>2%</div><div><div></div><div>86%</div><div></div><div>5%</div><div>9%</div></div></div>
1	E	348	<div><div>5%</div><div><div></div><div>81%</div><div></div><div>8%</div><div>10%</div></div></div>
1	F	348	<div><div>%</div><div><div></div><div>85%</div><div></div><div>5%</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	348	
1	H	348	

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	GOL	A	401	-	-	-	X
2	GOL	E	502	-	-	-	X
2	GOL	G	503	-	-	-	X
3	MES	E	501	-	-	-	X
3	MES	F	501	-	-	-	X
4	SO4	C	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20143 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 Beta-glucosidase-related glycosidases.

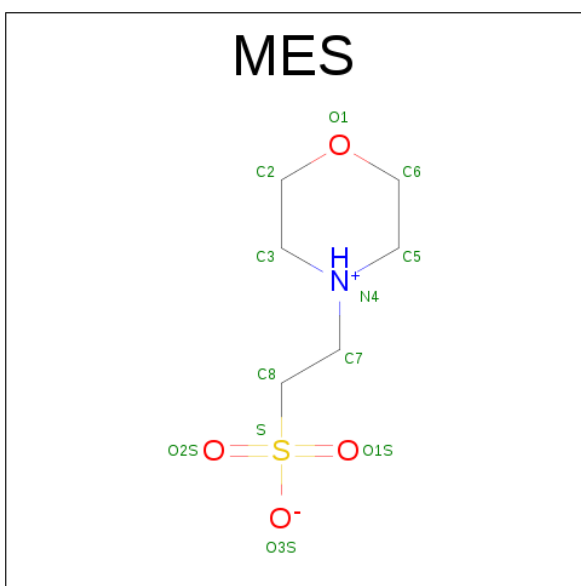
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	Se	0	1	0
			2317	1460	386	463	8			
1	B	313	Total	C	N	O	Se	0	2	0
			2331	1468	388	467	8			
1	C	321	Total	C	N	O	Se	0	2	0
			2363	1486	397	472	8			
1	D	316	Total	C	N	O	Se	0	2	0
			2334	1472	388	466	8			
1	E	312	Total	C	N	O	Se	0	1	0
			2300	1448	384	460	8			
1	F	313	Total	C	N	O	Se	0	0	0
			2311	1457	386	460	8			
1	G	323	Total	C	N	O	Se	0	2	0
			2380	1497	401	474	8			
1	H	309	Total	C	N	O	Se	0	0	0
			2281	1437	379	457	8			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



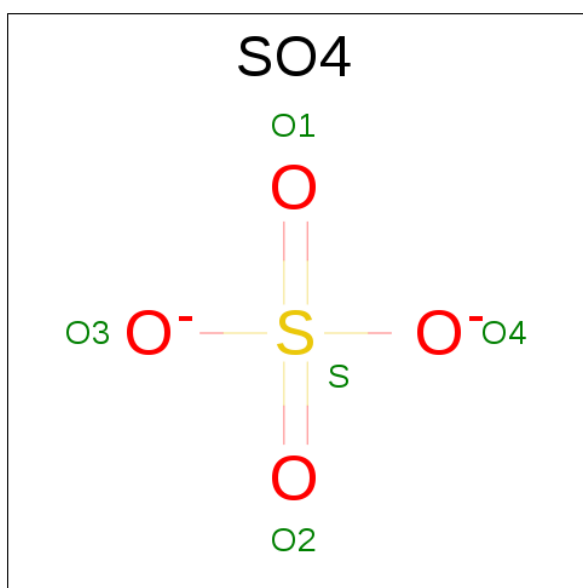
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		

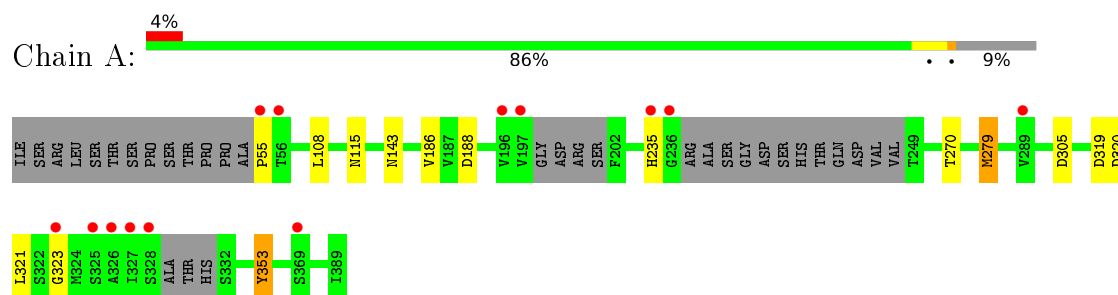
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total 173	O 173	0	0
6	B	181	Total 181	O 181	0	0
6	C	215	Total 215	O 215	0	0
6	D	186	Total 186	O 186	0	0
6	E	155	Total 155	O 155	0	0
6	F	198	Total 198	O 198	0	0
6	G	192	Total 192	O 192	0	0
6	H	143	Total 143	O 143	0	0

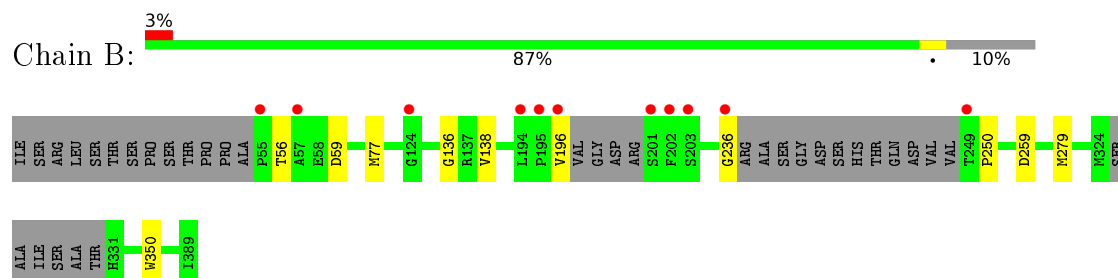
3 Residue-property plots

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

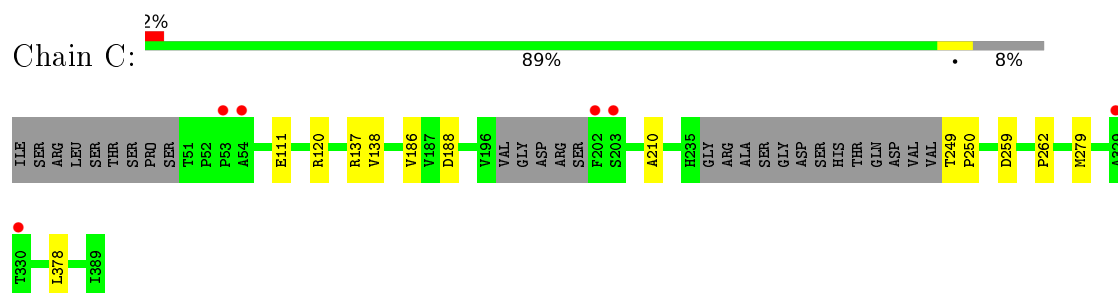
- Molecule 1: Beta-glucosidase-related glycosidases



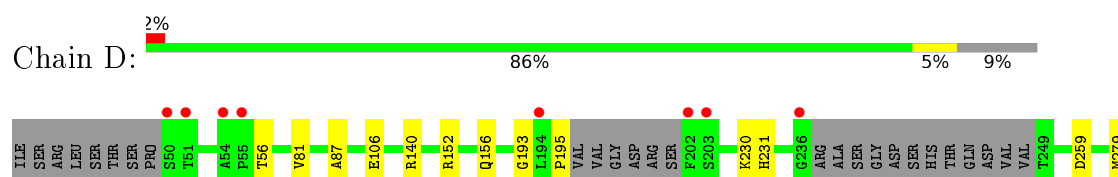
- Molecule 1: Beta-glucosidase-related glycosidases

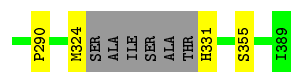


- Molecule 1: Beta-glucosidase-related glycosidases

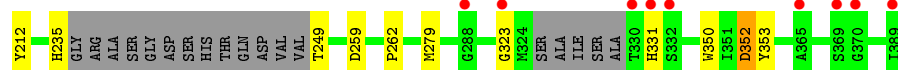
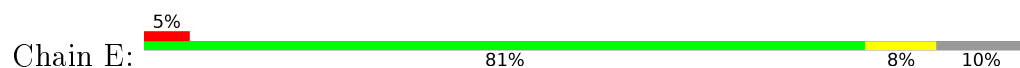


- Molecule 1: Beta-glucosidase-related glycosidases

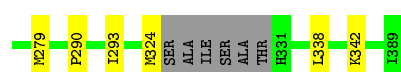
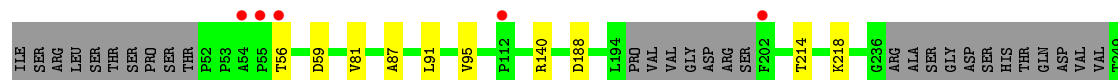
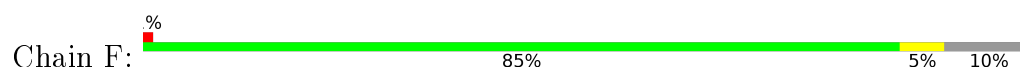




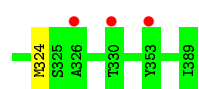
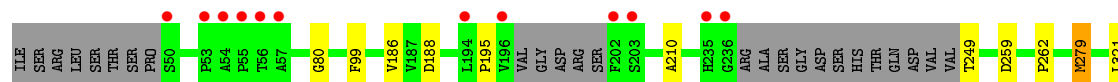
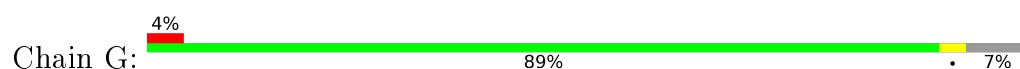
- Molecule 1: Beta-glucosidase-related glycosidases



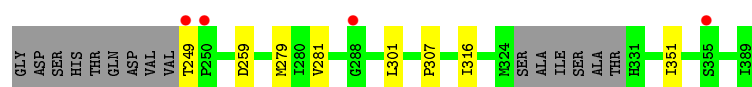
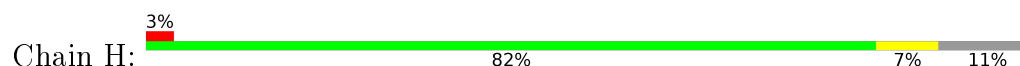
- Molecule 1: Beta-glucosidase-related glycosidases



- Molecule 1: Beta-glucosidase-related glycosidases



- Molecule 1: Beta-glucosidase-related glycosidases



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	308.07Å 91.36Å 120.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.28 – 2.25 37.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	84.1 (37.28-2.25) 96.6 (37.28-2.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.257 0.210 , 0.257	Depositor DCC
R_{free} test set	7758 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20143	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5901e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GOL, SO4, MES, CL

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	0.29	0/2352	0.51	1/3196 (0.0%)
1	B	0.30	0/2369	0.49	0/3218
1	C	0.30	0/2402	0.49	0/3268
1	D	0.31	0/2373	0.50	1/3227 (0.0%)
1	E	0.31	0/2335	0.49	2/3171 (0.1%)
1	F	0.30	0/2350	0.46	0/3193
1	G	0.29	0/2420	0.48	1/3292 (0.0%)
1	H	0.29	0/2317	0.48	1/3147 (0.0%)
All	All	0.30	0/18918	0.49	6/25712 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	55	PRO	N-CA-CB	5.94	110.43	103.30
1	E	55	PRO	N-CA-CB	5.92	110.40	103.30
1	A	55	PRO	N-CA-CB	5.89	110.38	103.30
1	E	195	PRO	N-CA-CB	5.88	110.35	103.30
1	D	195	PRO	N-CA-CB	5.73	110.18	103.30
1	G	195	PRO	N-CA-CB	5.42	109.80	103.30

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	2317	0	2220	7	0
1	B	2331	0	2249	5	0
1	C	2363	0	2275	10	0
1	D	2334	0	2233	9	0
1	E	2300	0	2203	15	0
1	F	2311	0	2232	9	0
1	G	2380	0	2287	7	0
1	H	2281	0	2196	11	0
2	A	6	0	8	0	0
2	C	6	0	8	3	0
2	E	6	0	8	0	0
2	G	6	0	8	0	0
3	C	12	0	12	0	0
3	D	12	0	12	1	0
3	E	12	0	12	1	0
3	F	12	0	12	1	0
4	C	5	0	0	0	0
4	G	5	0	0	0	0
5	G	1	0	0	0	0
6	A	173	0	0	1	0
6	B	181	0	0	0	0
6	C	215	0	0	2	0
6	D	186	0	0	2	0
6	E	155	0	0	6	0
6	F	198	0	0	2	0
6	G	192	0	0	1	0
6	H	143	0	0	1	0
All	All	20143	0	17975	74	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 2.

All (74) 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:C:120[A]:ARG:NH1	6:C:601:HOH:O	2.18	0.77
1:G:249:THR:N	6:G:601:HOH:O	2.23	0.71
1:H:259:ASP:OD2	6:H:401:HOH:O	2.14	0.65
1:E:202:PHE:N	6:E:1203:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:ASP:OD2	6:F:601:HOH:O	2.14	0.65
1:F:140:ARG:NH1	6:F:604:HOH:O	2.29	0.64
1:C:138:VAL:H	2:C:503:GOL:H12	1.62	0.64
1:D:156:GLN:OE1	6:D:601:HOH:O	2.16	0.63
1:A:235:HIS:HA	1:A:279:MSE:HE2	1.84	0.60
1:C:137:ARG:HE	2:C:503:GOL:H2	1.67	0.58
1:D:152:ARG:NH1	1:D:193:GLY:O	2.37	0.58
1:A:353:TYR:HB3	6:A:504:HOH:O	2.04	0.57
1:F:290:PRO:HB2	1:F:324:MSE:HE2	1.85	0.56
1:C:138:VAL:HG22	2:C:503:GOL:H12	1.86	0.56
1:D:331:HIS:N	6:D:605:HOH:O	2.38	0.56
1:D:259[B]:ASP:OD1	1:D:259[B]:ASP:N	2.37	0.56
1:E:186:VAL:HG12	1:E:188:ASP:H	1.70	0.56
1:E:352:ASP:OD1	6:E:1201:HOH:O	2.18	0.55
1:H:301:LEU:HD23	1:H:316:ILE:HD13	1.89	0.55
1:H:81:VAL:HG11	1:H:87:ALA:HA	1.88	0.55
1:G:259[B]:ASP:OD1	1:G:259[B]:ASP:N	2.40	0.54
1:G:321:LEU:HD22	1:G:324:MSE:HE2	1.88	0.54
1:E:125:ARG:NH1	6:E:1210:HOH:O	2.42	0.53
1:C:259[B]:ASP:N	1:C:259[B]:ASP:OD1	2.39	0.52
1:F:81:VAL:HG21	1:F:87:ALA:HB2	1.92	0.52
1:B:259[B]:ASP:OD1	1:B:259[B]:ASP:N	2.42	0.51
1:C:111:GLU:OE1	6:C:602:HOH:O	2.19	0.51
1:G:186:VAL:HG12	1:G:188:ASP:H	1.77	0.50
1:E:249:THR:N	6:E:1211:HOH:O	2.45	0.50
1:H:68:GLN:O	1:H:72:GLN:HG3	2.12	0.49
1:E:155:ALA:HA	1:E:212:TYR:CE2	2.47	0.49
1:H:152:ARG:NH2	1:H:194:LEU:O	2.45	0.49
1:H:249:THR:HG21	1:H:281:VAL:HG22	1.95	0.49
1:A:319:ASP:OD1	1:A:320:ASP:N	2.46	0.47
1:A:279:MSE:H	1:A:279:MSE:SE	2.48	0.47
1:B:56:THR:HG22	1:B:59:ASP:H	1.79	0.47
1:E:259[B]:ASP:OD1	1:E:259[B]:ASP:N	2.48	0.46
1:A:186:VAL:HG12	1:A:188:ASP:H	1.81	0.46
1:H:123:VAL:HG12	1:H:125:ARG:HG2	1.98	0.46
1:F:338:LEU:HG	1:F:342:LYS:HD2	1.98	0.46
1:B:77:MSE:HB3	1:B:350:TRP:HZ3	1.81	0.46
1:G:210:ALA:HB2	1:G:262:PRO:HA	1.98	0.46
1:H:103:TRP:HZ2	1:H:351:ILE:HG12	1.81	0.45
1:F:293:ILE:HG23	1:F:324:MSE:HE1	1.97	0.45
1:A:108:LEU:O	1:A:115:ASN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:GLY:HA2	1:G:99:PHE:HB3	1.99	0.45
1:C:186:VAL:HG12	1:C:188:ASP:H	1.82	0.45
1:E:235:HIS:O	6:E:1202:HOH:O	2.21	0.44
1:B:236:GLY:HA2	1:B:250:PRO:HG2	2.00	0.43
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.86	0.43
3:D:501:MES:H51	3:D:501:MES:H81	1.62	0.43
1:F:56:THR:HG23	1:F:59:ASP:H	1.84	0.43
1:G:279:MSE:SE	1:G:279:MSE:H	2.52	0.43
3:F:501:MES:O3S	1:H:307:PRO:HD3	2.19	0.43
1:D:290:PRO:HB2	1:D:324:MSE:HE2	2.00	0.43
1:A:143:ASN:O	1:B:136:GLY:HA2	2.19	0.42
1:E:140:ARG:HD3	6:E:1283:HOH:O	2.20	0.42
1:H:102:SER:HA	1:H:139:GLN:HB2	2.00	0.42
1:D:81:VAL:HG11	1:D:87:ALA:HA	2.02	0.42
1:C:249:THR:HA	1:C:250:PRO:HD3	1.94	0.41
1:E:145:LEU:HD13	1:E:174:LEU:HD12	2.02	0.41
3:E:501:MES:H51	3:E:501:MES:H81	1.75	0.41
1:D:230:LYS:HA	1:D:231:HIS:HA	1.86	0.41
1:E:95:VAL:O	1:E:125:ARG:NH2	2.50	0.41
1:F:214:THR:HG22	1:F:218:LYS:HE3	2.03	0.41
1:E:210:ALA:HB2	1:E:262:PRO:HA	2.03	0.41
1:E:80:GLY:HA2	1:E:99:PHE:HB3	2.03	0.41
1:E:108:LEU:O	1:E:115:ASN:HA	2.21	0.41
1:D:81:VAL:HG21	1:D:87:ALA:HB2	2.03	0.41
1:F:91:LEU:HA	1:F:95:VAL:HG12	2.03	0.41
1:C:210:ALA:HB2	1:C:262:PRO:HA	2.03	0.40
1:E:79:VAL:HA	1:E:350:TRP:O	2.22	0.40
1:D:106:GLU:HG3	1:D:140:ARG:HB3	2.02	0.40
1:H:80:GLY:HA2	1:H:99:PHE:HB3	2.03	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	309/348 (89%)	302 (98%)	6 (2%)	1 (0%)	46	52
1	B	307/348 (88%)	300 (98%)	7 (2%)	0	100	100
1	C	317/348 (91%)	312 (98%)	5 (2%)	0	100	100
1	D	310/348 (89%)	305 (98%)	5 (2%)	0	100	100
1	E	305/348 (88%)	298 (98%)	6 (2%)	1 (0%)	46	52
1	F	305/348 (88%)	298 (98%)	7 (2%)	0	100	100
1	G	319/348 (92%)	315 (99%)	4 (1%)	0	100	100
1	H	301/348 (86%)	294 (98%)	7 (2%)	0	100	100
All	All	2473/2784 (89%)	2424 (98%)	47 (2%)	2 (0%)	56	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	323	GLY
1	A	323	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	235/264 (89%)	230 (98%)	5 (2%)	61	71
1	B	243/264 (92%)	240 (99%)	3 (1%)	78	87
1	C	243/264 (92%)	242 (100%)	1 (0%)	93	96
1	D	239/264 (90%)	236 (99%)	3 (1%)	76	85
1	E	235/264 (89%)	230 (98%)	5 (2%)	61	71
1	F	239/264 (90%)	238 (100%)	1 (0%)	93	96
1	G	244/264 (92%)	243 (100%)	1 (0%)	93	96
1	H	236/264 (89%)	231 (98%)	5 (2%)	61	71
All	All	1914/2112 (91%)	1890 (99%)	24 (1%)	76	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	THR
1	A	279	MSE
1	A	305	ASP
1	A	321	LEU
1	A	353	TYR
1	B	138	VAL
1	B	196	VAL
1	B	279	MSE
1	C	279	MSE
1	D	56	THR
1	D	279	MSE
1	D	355	SER
1	E	70	ARG
1	E	279	MSE
1	E	331	HIS
1	E	352	ASP
1	E	353	TYR
1	F	279	MSE
1	G	279	MSE
1	H	56	THR
1	H	95	VAL
1	H	138	VAL
1	H	152	ARG
1	H	279	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 11 ligands modelled in this entry, 1 is 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$
2	GOL	A	401	-	5,5,5	0.31	0	5,5,5	0.27	0
3	MES	C	501	-	12,12,12	2.25	1 (8%)	15,16,16	2.95	8 (53%)
4	SO4	C	502	-	4,4,4	0.21	0	6,6,6	0.21	0
2	GOL	C	503	-	5,5,5	0.39	0	5,5,5	0.19	0
3	MES	D	501	-	12,12,12	2.22	1 (8%)	15,16,16	2.53	6 (40%)
3	MES	E	501	-	12,12,12	2.19	1 (8%)	15,16,16	2.33	5 (33%)
2	GOL	E	502	-	5,5,5	0.40	0	5,5,5	0.23	0
3	MES	F	501	-	12,12,12	2.29	1 (8%)	15,16,16	2.43	7 (46%)
4	SO4	G	501	-	4,4,4	0.22	0	6,6,6	0.10	0
2	GOL	G	503	-	5,5,5	0.36	0	5,5,5	0.16	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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
3	MES	C	501	-	-	0/6/14/14	0/1/1/1
4	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
3	MES	D	501	-	-	0/6/14/14	0/1/1/1
3	MES	E	501	-	-	0/6/14/14	0/1/1/1
2	GOL	E	502	-	-	0/4/4/4	0/0/0/0
3	MES	F	501	-	-	0/6/14/14	0/1/1/1
4	SO4	G	501	-	-	0/0/0/0	0/0/0/0
2	GOL	G	503	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	MES	C8-S	-7.60	1.66	1.77
3	C	501	MES	C8-S	-7.59	1.66	1.77
3	D	501	MES	C8-S	-7.46	1.66	1.77
3	E	501	MES	C8-S	-7.35	1.66	1.77

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	MES	C2-C3-N4	-2.99	105.54	110.11
3	C	501	MES	C2-C3-N4	-2.67	106.03	110.11
3	C	501	MES	C6-C5-N4	-2.50	106.29	110.11
3	D	501	MES	O2S-S-O1S	-2.20	107.73	113.96
3	E	501	MES	C6-C5-N4	-2.12	106.87	110.11
3	F	501	MES	C6-C5-N4	-2.12	106.88	110.11
3	C	501	MES	O2S-S-O1S	-2.05	108.16	113.96
3	D	501	MES	C7-N4-C3	2.14	115.91	111.25
3	E	501	MES	C7-N4-C5	2.31	116.28	111.25
3	D	501	MES	C7-N4-C5	2.32	116.29	111.25
3	F	501	MES	C7-N4-C5	2.54	116.77	111.25
3	F	501	MES	C7-N4-C3	2.67	117.07	111.25
3	C	501	MES	C7-N4-C5	3.12	118.04	111.25
3	C	501	MES	C7-N4-C3	3.14	118.09	111.25
3	D	501	MES	O1S-S-C8	3.55	109.38	106.87
3	F	501	MES	O2S-S-C8	3.58	109.40	106.87
3	E	501	MES	O1S-S-C8	3.70	109.48	106.87
3	F	501	MES	C5-N4-C3	4.23	118.35	108.87
3	F	501	MES	O1S-S-C8	4.28	109.89	106.87
3	E	501	MES	O2S-S-C8	4.71	110.20	106.87
3	E	501	MES	C5-N4-C3	4.78	119.57	108.87
3	C	501	MES	O2S-S-C8	5.10	110.47	106.87
3	C	501	MES	O1S-S-C8	5.23	110.57	106.87
3	D	501	MES	C5-N4-C3	5.24	120.61	108.87
3	C	501	MES	C5-N4-C3	5.77	121.80	108.87
3	D	501	MES	O2S-S-C8	5.85	111.00	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	MES	1	0
3	E	501	MES	1	0
3	F	501	MES	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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	308/348 (88%)	-0.15	13 (4%) 40 44	23, 37, 70, 140	0
1	B	305/348 (87%)	-0.18	11 (3%) 46 50	23, 34, 66, 112	0
1	C	313/348 (89%)	-0.24	6 (1%) 70 74	19, 33, 64, 74	0
1	D	308/348 (88%)	-0.30	8 (2%) 59 63	19, 31, 66, 96	0
1	E	304/348 (87%)	-0.04	16 (5%) 30 33	29, 41, 75, 117	0
1	F	305/348 (87%)	-0.29	5 (1%) 74 77	27, 38, 73, 110	0
1	G	315/348 (90%)	-0.08	15 (4%) 34 38	28, 39, 73, 114	0
1	H	301/348 (86%)	-0.06	11 (3%) 45 49	31, 41, 73, 115	0
All	All	2459/2784 (88%)	-0.17	85 (3%) 48 52	19, 38, 71, 140	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	ALA	9.2
1	H	55	PRO	7.1
1	B	55	PRO	6.2
1	D	55	PRO	5.7
1	D	202	PHE	5.5
1	G	50	SER	5.3
1	A	197	VAL	5.2
1	G	53	PRO	4.9
1	B	202	PHE	4.9
1	B	194	LEU	4.8
1	F	55	PRO	4.7
1	B	203	SER	4.6
1	B	196	VAL	4.4
1	B	201	SER	4.3
1	E	55	PRO	4.3
1	A	196	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	330	THR	4.2
1	F	54	ALA	4.2
1	E	323	GLY	4.2
1	D	51	THR	4.1
1	C	330	THR	4.1
1	G	236	GLY	3.9
1	D	194	LEU	3.8
1	G	56	THR	3.7
1	A	55	PRO	3.7
1	G	57	ALA	3.7
1	A	325	SER	3.6
1	E	365	ALA	3.5
1	C	202	PHE	3.4
1	G	353	TYR	3.4
1	A	327	ILE	3.4
1	B	249	THR	3.2
1	G	235	HIS	3.2
1	E	369	SER	3.1
1	B	236	GLY	3.1
1	E	202	PHE	3.1
1	G	196	VAL	3.0
1	B	57	ALA	3.0
1	G	54	ALA	3.0
1	H	249	THR	3.0
1	E	331	HIS	3.0
1	H	250	PRO	3.0
1	H	121	GLU	2.9
1	F	202	PHE	2.9
1	C	53	PRO	2.9
1	E	124	GLY	2.9
1	E	288	GLY	2.9
1	D	54	ALA	2.8
1	C	203	SER	2.8
1	D	50	SER	2.8
1	D	203	SER	2.7
1	G	194	LEU	2.7
1	A	328	SER	2.7
1	H	57	ALA	2.7
1	E	332	SER	2.6
1	H	67	GLU	2.6
1	A	56	THR	2.6
1	A	236	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	56	THR	2.6
1	C	329	ALA	2.6
1	F	56	THR	2.5
1	F	112	PRO	2.5
1	H	68	GLN	2.5
1	E	57	ALA	2.4
1	E	67	GLU	2.4
1	D	236	GLY	2.4
1	G	55	PRO	2.4
1	G	326	ALA	2.4
1	E	389	ILE	2.3
1	E	60	LEU	2.3
1	H	202	PHE	2.3
1	A	289	VAL	2.3
1	H	288	GLY	2.2
1	B	195	PRO	2.2
1	B	124	GLY	2.2
1	E	370	GLY	2.2
1	G	203	SER	2.1
1	H	355	SER	2.1
1	C	54	ALA	2.1
1	G	202	PHE	2.1
1	A	323	GLY	2.1
1	A	369	SER	2.1
1	A	235	HIS	2.0
1	H	56	THR	2.0
1	E	330	THR	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, 95th 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 ²)	Q<0.9
2	GOL	G	503	6/6	0.80	0.36	19.21	54,67,75,77	0
4	SO4	C	502	5/5	0.80	0.24	6.29	80,90,98,101	0
2	GOL	E	502	6/6	0.90	0.27	6.15	51,62,68,68	0
2	GOL	A	401	6/6	0.84	0.23	4.03	46,55,62,64	0
3	MES	F	501	12/12	0.94	0.16	2.35	60,66,75,80	0
3	MES	E	501	12/12	0.94	0.17	2.24	57,76,83,83	0
3	MES	C	501	12/12	0.97	0.15	1.24	42,56,62,64	0
3	MES	D	501	12/12	0.96	0.12	1.22	52,57,60,62	0
4	SO4	G	501	5/5	0.86	0.22	0.65	120,123,124,126	0
5	CL	G	502	1/1	0.96	0.06	-1.56	57,57,57,57	0
2	GOL	C	503	6/6	0.89	0.24	-	56,61,70,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.