



Full wwPDB X-ray Structure Validation Report

May 29, 2020 – 03:52 pm BST


PDB ID : 2R5S
Title : The crystal structure of a domain of protein VP0806 (unknown function) from *Vibrio parahaemolyticus* RIMD 2210633
Authors : Tan, K.; Wu, R.; Abdullah, J.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-09-04
Resolution : 2.14 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

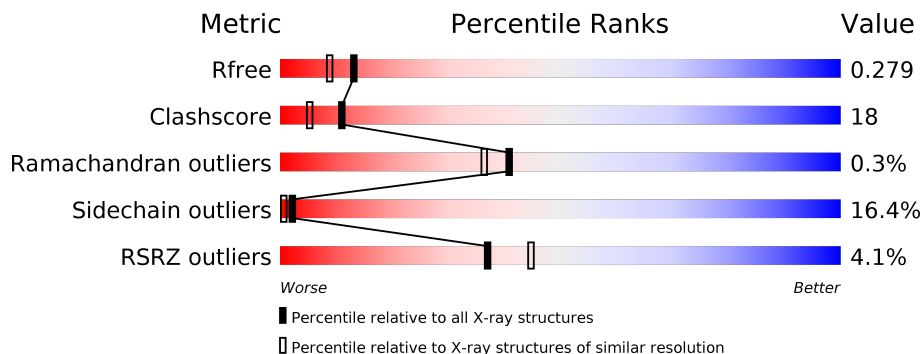
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	176	 3% 58% 32% 7% •
1	B	176	 5% 64% 24% 9% ••

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	EDO	A	2	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2850 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.

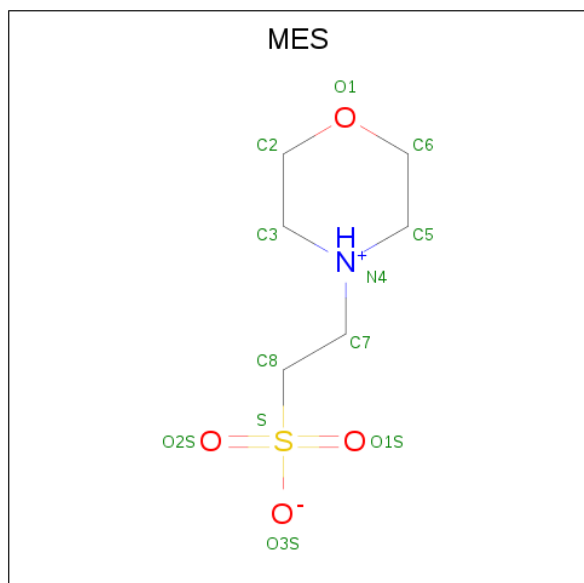
- Molecule 1 is a protein called Uncharacterized protein VP0806.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	171	1370	864	229	274	2	1	0	2	0
1	B	171	1356	853	228	272	2	1	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

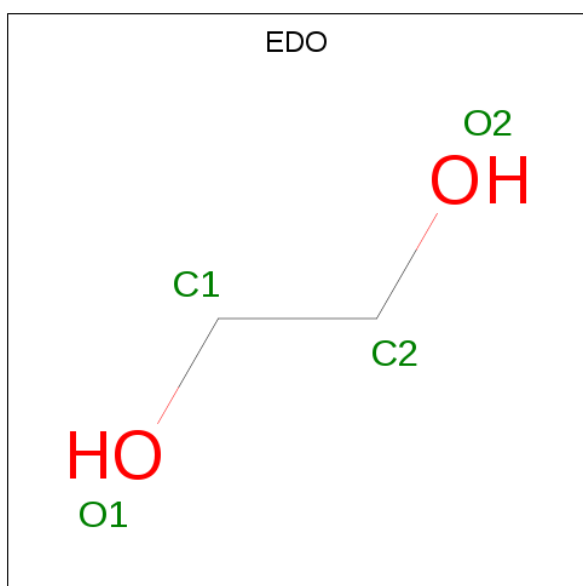
Chain	Residue	Modelled	Actual	Comment	Reference
A	109	SER	-	EXPRESSION TAG	UNP Q87RI8
A	110	ASN	-	EXPRESSION TAG	UNP Q87RI8
A	111	ALA	-	EXPRESSION TAG	UNP Q87RI8
B	109	SER	-	EXPRESSION TAG	UNP Q87RI8
B	110	ASN	-	EXPRESSION TAG	UNP Q87RI8
B	111	ALA	-	EXPRESSION TAG	UNP Q87RI8

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



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

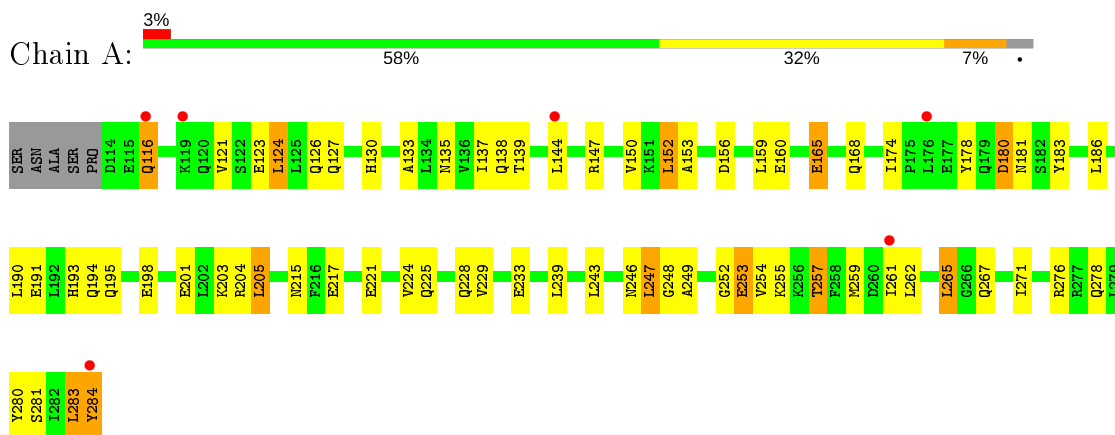
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	29	Total	O	0	0
			29	29		

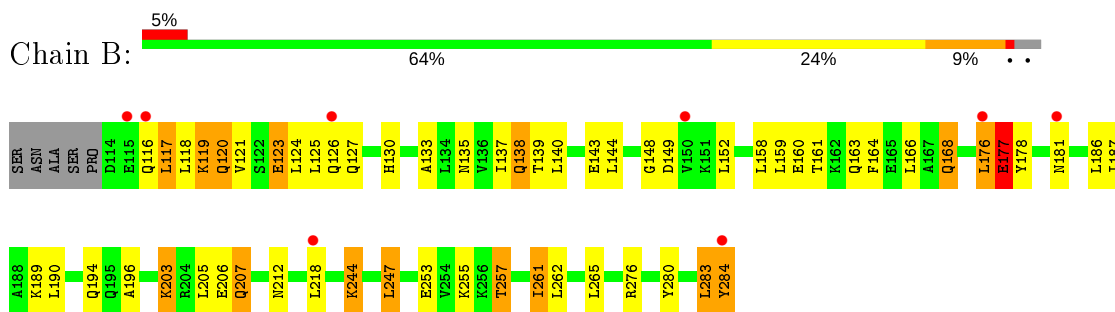
3 Residue-property plots [i](#)

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: Uncharacterized protein VP0806



- Molecule 1: Uncharacterized protein VP0806



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	53.00Å 116.48Å 62.22Å 90.00° 88.75° 90.00°	Depositor
Resolution (Å)	29.12 – 2.14 29.12 – 2.14	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.12-2.14) 90.0 (29.12-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.279 0.220 , 0.279	Depositor DCC
R_{free} test set	1011 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtrriage
Anisotropy	0.574	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.329 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2850	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, MES, ACT

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	0.97	2/1390 (0.1%)	0.99	1/1874 (0.1%)
1	B	1.05	1/1370 (0.1%)	1.06	2/1848 (0.1%)
All	All	1.01	3/2760 (0.1%)	1.02	3/3722 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLU	CB-CG	-5.53	1.41	1.52
1	A	253	GLU	CG-CD	5.24	1.59	1.51
1	B	177	GLU	CG-CD	-5.21	1.44	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	LYS	CD-CE-NZ	-5.47	99.11	111.70
1	A	124	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	176	LEU	CA-CB-CG	5.32	127.55	115.30

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	1370	0	1374	52	1
1	B	1356	0	1359	52	1
2	A	12	0	12	1	0
2	B	36	0	36	0	0
3	A	8	0	12	7	0
3	B	4	0	6	0	0
4	B	4	0	3	1	0
5	A	31	0	0	4	0
5	B	29	0	0	1	0
All	All	2850	0	2802	101	1

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 18.

All (101) 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:B:161:THR:HG23	1:B:163:GLN:HG3	1.39	1.00
1:A:281:SER:HB3	3:A:2:EDO:H21	1.46	0.98
1:A:224:VAL:O	1:A:228:GLN:HG3	1.67	0.94
1:A:168:GLN:HB2	1:A:190:LEU:HD21	1.46	0.93
1:A:123:GLU:O	1:A:127:GLN:HG3	1.74	0.87
1:A:252:GLY:HA2	5:A:288:HOH:O	1.78	0.83
1:A:281:SER:CB	3:A:2:EDO:H21	2.08	0.83
1:B:158:LEU:O	1:B:161:THR:HG22	1.79	0.81
1:A:281:SER:HB3	3:A:2:EDO:C2	2.15	0.77
1:B:168:GLN:HG2	1:B:190:LEU:HD21	1.64	0.77
1:B:117:LEU:HD23	1:B:117:LEU:H	1.47	0.77
1:B:133:ALA:O	1:B:137:ILE:HG12	1.87	0.74
1:A:243:LEU:HD21	1:A:254:VAL:HG12	1.71	0.72
1:A:204:ARG:NH2	1:A:205:LEU:HD13	2.04	0.72
1:B:161:THR:CG2	1:B:163:GLN:HE21	2.04	0.70
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.56	0.70
1:A:168:GLN:CB	1:A:190:LEU:HD21	2.23	0.68
1:B:164:PHE:O	1:B:168:GLN:HB2	1.94	0.68
1:A:278:GLN:HA	5:A:315:HOH:O	1.94	0.67
1:B:190:LEU:O	1:B:194:GLN:HG3	1.95	0.67
1:A:217:GLU:O	1:A:221:GLU:HG3	1.94	0.66
1:A:283:LEU:HD23	1:B:189:LYS:HG3	1.78	0.66
1:A:133:ALA:O	1:A:137:ILE:HG12	1.97	0.65
1:A:152:LEU:HD13	1:A:174:ILE:HD12	1.79	0.64
1:A:281:SER:CA	3:A:2:EDO:H21	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:VAL:HG11	1:B:137:ILE:HD11	1.78	0.64
1:A:247:LEU:HD23	1:A:284[B]:TYR:CE2	2.32	0.64
1:A:130:HIS:CE1	1:A:160:GLU:HG3	2.34	0.62
1:A:257:THR:O	1:A:261:ILE:HD13	2.00	0.61
1:B:280:TYR:HA	1:B:283:LEU:HD22	1.82	0.61
1:A:243:LEU:CD2	1:A:254:VAL:HG12	2.31	0.60
1:B:203:LYS:NZ	1:B:206:GLU:OE2	2.36	0.58
1:B:161:THR:CG2	1:B:163:GLN:HG3	2.25	0.57
1:A:280:TYR:HA	1:A:283:LEU:HD22	1.86	0.57
1:A:229:VAL:HG12	3:A:3:EDO:H22	1.87	0.57
1:B:203:LYS:O	1:B:207:GLN:HG2	2.03	0.56
1:A:135:ASN:O	1:A:139:THR:HG23	2.05	0.56
1:A:262:LEU:HD13	1:A:276:ARG:HG2	1.87	0.56
1:A:204:ARG:NH2	1:A:205:LEU:CD1	2.68	0.56
1:B:161:THR:HG21	1:B:163:GLN:HE21	1.71	0.56
1:A:284[A]:TYR:HD2	1:B:181:ASN:ND2	2.04	0.55
1:A:253:GLU:O	1:A:257:THR:HG22	2.07	0.55
1:B:161:THR:HG23	1:B:163:GLN:HE21	1.70	0.54
1:A:191:GLU:O	1:A:195:GLN:HG3	2.07	0.54
1:B:161:THR:HG23	1:B:163:GLN:CG	2.25	0.54
1:B:253:GLU:O	1:B:257:THR:CG2	2.57	0.53
1:B:161:THR:CG2	1:B:163:GLN:NE2	2.73	0.51
1:B:207:GLN:CA	1:B:207:GLN:HE21	2.23	0.51
1:B:135:ASN:O	1:B:139:THR:HG23	2.12	0.49
1:B:244:LYS:CE	4:B:1:ACT:H2	2.43	0.49
1:A:281:SER:HA	3:A:2:EDO:H21	1.94	0.49
2:A:4:MES:H71	5:A:287:HOH:O	2.12	0.49
1:A:284[A]:TYR:CD2	1:B:181:ASN:ND2	2.80	0.49
1:B:161:THR:HG21	1:B:163:GLN:NE2	2.26	0.49
1:A:253:GLU:O	1:A:257:THR:CG2	2.60	0.49
1:A:247:LEU:CD2	1:A:284[B]:TYR:CE2	2.97	0.47
1:A:267:GLN:NE2	1:B:196:ALA:HA	2.29	0.47
1:A:248:GLY:O	1:A:249:ALA:C	2.51	0.47
1:B:117:LEU:CD2	1:B:117:LEU:H	2.23	0.47
1:B:116:GLN:NE2	1:B:120:GLN:HE22	2.12	0.47
1:B:125:LEU:O	1:B:126:GLN:C	2.51	0.47
1:A:121:VAL:HG21	1:A:137:ILE:CD1	2.45	0.46
1:A:180:ASP:HB3	1:A:183:TYR:H	1.78	0.46
1:B:253:GLU:O	1:B:257:THR:HG23	2.15	0.46
1:A:243:LEU:HD21	1:A:255:LYS:N	2.31	0.46
1:B:177:GLU:HG3	1:B:177:GLU:H	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:HIS:ND1	3:A:3:EDO:H12	2.31	0.46
1:B:116:GLN:HG2	1:B:116:GLN:O	2.14	0.46
1:A:233:GLU:HG3	1:A:271:ILE:HD12	1.98	0.46
1:B:116:GLN:HG2	1:B:119:LYS:HB3	1.99	0.45
1:B:117:LEU:HA	1:B:120:GLN:HB2	1.98	0.45
1:B:148:GLY:HA3	1:B:178:TYR:CD2	2.52	0.45
1:A:121:VAL:HG21	1:A:137:ILE:HD13	1.98	0.44
1:B:121:VAL:HG21	1:B:137:ILE:HD13	1.99	0.44
1:B:121:VAL:CG1	1:B:137:ILE:HD11	2.47	0.44
1:B:253:GLU:O	1:B:257:THR:HG22	2.18	0.43
1:A:201:GLU:OE2	1:A:204:ARG:NH2	2.42	0.43
1:B:123:GLU:O	1:B:127:GLN:HG3	2.17	0.43
1:B:247:LEU:HD22	5:B:294:HOH:O	2.17	0.43
1:A:225:GLN:OE1	1:A:225:GLN:HA	2.19	0.43
1:B:138:GLN:HB2	1:B:138:GLN:HE21	1.61	0.43
1:B:261:ILE:CD1	1:B:261:ILE:N	2.81	0.43
1:B:284:TYR:C	1:B:284:TYR:HD2	2.21	0.43
1:A:255:LYS:O	1:A:259:MSE:HG2	2.18	0.43
1:B:149:ASP:OD1	1:B:149:ASP:N	2.52	0.43
1:B:118:LEU:HG	1:B:144:LEU:HD21	2.01	0.43
1:B:130:HIS:CE1	1:B:160:GLU:HG3	2.55	0.42
1:B:284:TYR:C	1:B:284:TYR:CD2	2.93	0.42
1:B:262:LEU:HD13	1:B:276:ARG:HG2	2.02	0.42
1:A:156:ASP:O	1:A:160:GLU:HG2	2.20	0.42
1:B:118:LEU:HD11	1:B:144:LEU:HD11	2.00	0.42
1:A:265:LEU:HA	1:A:265:LEU:HD12	1.78	0.42
1:A:150:VAL:O	1:A:153:ALA:HB3	2.20	0.41
1:B:262:LEU:HD13	1:B:276:ARG:CG	2.50	0.41
1:B:257:THR:O	1:B:261:ILE:HD13	2.21	0.41
1:A:144:LEU:HD12	1:A:147:ARG:HD3	2.03	0.40
1:A:116:GLN:N	5:A:301:HOH:O	2.45	0.40
1:A:190:LEU:O	1:A:194:GLN:HG2	2.22	0.40
1:A:123:GLU:O	1:A:127:GLN:CG	2.58	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:OH	1:B:178:TYR:OH[4_556]	1.87	0.33

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	170/176 (97%)	160 (94%)	9 (5%)	1 (1%)	25	17
1	B	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
All	All	339/352 (96%)	324 (96%)	14 (4%)	1 (0%)	41	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ASN

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	148/149 (99%)	126 (85%)	22 (15%)	3	1
1	B	146/149 (98%)	118 (81%)	28 (19%)	1	0
All	All	294/298 (99%)	244 (83%)	50 (17%)	2	0

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

Mol	Chain	Res	Type
1	A	116	GLN
1	A	124	LEU
1	A	126	GLN
1	A	138	GLN
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	165	GLU
1	A	180	ASP
1	A	181[A]	ASN
1	A	181[B]	ASN
1	A	186	LEU
1	A	198	GLU
1	A	203	LYS
1	A	205	LEU
1	A	239	LEU
1	A	246	ASN
1	A	247	LEU
1	A	257	THR
1	A	265	LEU
1	A	283	LEU
1	A	284[A]	TYR
1	A	284[B]	TYR
1	B	117	LEU
1	B	119	LYS
1	B	120	GLN
1	B	123	GLU
1	B	124	LEU
1	B	138	GLN
1	B	140	LEU
1	B	143	GLU
1	B	152	LEU
1	B	159	LEU
1	B	166	LEU
1	B	168	GLN
1	B	176	LEU
1	B	177	GLU
1	B	186	LEU
1	B	187	ILE
1	B	203	LYS
1	B	205	LEU
1	B	207	GLN
1	B	212	ASN
1	B	218	LEU
1	B	247	LEU
1	B	255	LYS
1	B	257	THR
1	B	261	ILE

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Mol	Chain	Res	Type
1	B	265	LEU
1	B	283	LEU
1	B	284	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	246	ASN
1	A	267	GLN
1	B	116	GLN
1	B	130	HIS
1	B	138	GLN
1	B	163	GLN
1	B	195	GLN
1	B	207	GLN
1	B	241	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](#)

8 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	MES	B	3	-	12,12,12	1.90	1 (8%)	14,16,16	2.52	6 (42%)
3	EDO	B	286	-	3,3,3	0.76	0	2,2,2	0.24	0
4	ACT	B	1	-	1,3,3	2.83	1 (100%)	0,3,3	0.00	-
2	MES	B	285	-	12,12,12	2.13	1 (8%)	14,16,16	2.81	8 (57%)
2	MES	A	4	-	12,12,12	2.16	1 (8%)	14,16,16	2.55	7 (50%)
2	MES	B	2	-	12,12,12	1.68	1 (8%)	14,16,16	2.53	7 (50%)
3	EDO	A	2	-	3,3,3	0.50	0	2,2,2	0.12	0
3	EDO	A	3	-	3,3,3	0.60	0	2,2,2	0.26	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	MES	B	3	-	-	4/6/14/14	0/1/1/1
3	EDO	B	286	-	-	1/1/1/1	-
2	MES	B	285	-	-	5/6/14/14	0/1/1/1
2	MES	A	4	-	-	2/6/14/14	0/1/1/1
2	MES	B	2	-	-	4/6/14/14	0/1/1/1
3	EDO	A	2	-	-	1/1/1/1	-
3	EDO	A	3	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4	MES	C8-S	-7.04	1.67	1.77
2	B	285	MES	C8-S	-6.68	1.68	1.77
2	B	3	MES	C8-S	-5.98	1.69	1.77
2	B	2	MES	C8-S	-5.22	1.70	1.77
4	B	1	ACT	CH3-C	2.83	1.52	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	MES	C5-N4-C3	6.35	123.13	108.83
2	B	285	MES	C5-N4-C3	5.16	120.44	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	MES	C5-N4-C3	5.08	120.27	108.83
2	B	2	MES	C5-N4-C3	5.03	120.16	108.83
2	B	285	MES	C7-N4-C3	4.27	122.15	111.23
2	B	2	MES	O3S-S-C8	4.10	112.40	105.77
2	B	285	MES	O3S-S-C8	4.06	112.33	105.77
2	B	285	MES	C6-C5-N4	-3.83	104.29	110.10
2	A	4	MES	C7-N4-C3	3.81	120.97	111.23
2	B	2	MES	C7-N4-C3	3.60	120.44	111.23
2	B	2	MES	C7-N4-C5	3.19	119.41	111.23
2	B	3	MES	O2S-S-C8	3.13	110.68	106.92
2	B	285	MES	O1-C6-C5	-3.13	104.91	111.80
2	B	3	MES	C7-N4-C3	3.08	119.11	111.23
2	A	4	MES	C6-C5-N4	-2.98	105.58	110.10
2	A	4	MES	C7-N4-C5	2.94	118.75	111.23
2	A	4	MES	C2-C3-N4	-2.86	105.76	110.10
2	B	2	MES	C2-C3-N4	-2.86	105.77	110.10
2	A	4	MES	O1S-S-C8	2.80	110.28	106.92
2	B	3	MES	O1S-S-C8	2.76	110.23	106.92
2	A	4	MES	O2S-S-C8	2.59	110.03	106.92
2	B	3	MES	C7-N4-C5	2.54	117.74	111.23
2	B	285	MES	C7-N4-C5	2.41	117.41	111.23
2	B	2	MES	O1S-S-C8	2.40	109.81	106.92
2	B	285	MES	O1S-S-C8	2.38	109.78	106.92
2	B	2	MES	O1-C6-C5	-2.34	106.64	111.80
2	B	3	MES	C2-C3-N4	2.30	113.59	110.10
2	B	285	MES	O1-C2-C3	2.11	116.43	111.80

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MES	C8-C7-N4-C5
2	B	3	MES	C7-C8-S-O1S
2	B	285	MES	C8-C7-N4-C3
2	B	285	MES	C7-C8-S-O2S
2	B	285	MES	C7-C8-S-O3S
2	B	2	MES	C7-C8-S-O1S
2	B	2	MES	C7-C8-S-O2S
3	A	2	EDO	O1-C1-C2-O2
3	B	286	EDO	O1-C1-C2-O2
3	A	3	EDO	O1-C1-C2-O2
2	B	3	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
2	B	2	MES	C7-C8-S-O3S
2	A	4	MES	C8-C7-N4-C5
2	B	3	MES	C7-C8-S-O2S
2	B	285	MES	C7-C8-S-O1S
2	B	285	MES	C8-C7-N4-C5
2	B	2	MES	C8-C7-N4-C5
2	A	4	MES	N4-C7-C8-S

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	ACT	1	0
2	A	4	MES	1	0
3	A	2	EDO	5	0
3	A	3	EDO	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 [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, 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	170/176 (96%)	0.52	6 (3%) 44 51	44, 56, 65, 74	1 (0%)
1	B	170/176 (96%)	0.50	8 (4%) 31 38	46, 56, 65, 73	1 (0%)
All	All	340/352 (96%)	0.51	14 (4%) 37 45	44, 56, 65, 74	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284[A]	TYR	5.3
1	B	218	LEU	3.4
1	B	116	GLN	3.4
1	A	119	LYS	3.1
1	B	284	TYR	2.9
1	A	261	ILE	2.6
1	A	144	LEU	2.5
1	B	126	GLN	2.4
1	B	176	LEU	2.3
1	B	150	VAL	2.3
1	A	116	GLN	2.3
1	A	176	LEU	2.3
1	B	115	GLU	2.1
1	B	181	ASN	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. 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	B-factors(Å ²)	Q<0.9
2	MES	B	3	12/12	0.61	0.28	83,85,94,94	12
2	MES	B	285	12/12	0.68	0.22	65,69,88,88	0
4	ACT	B	1	4/4	0.74	0.25	64,64,64,66	0
2	MES	A	4	12/12	0.78	0.26	75,79,93,93	12
2	MES	B	2	12/12	0.82	0.24	64,67,85,86	12
3	EDO	B	286	4/4	0.83	0.17	72,73,74,75	0
3	EDO	A	3	4/4	0.83	0.33	66,68,68,69	0
3	EDO	A	2	4/4	0.84	0.45	59,59,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.