Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 02:32 AM EDT

PDB ID	:	5EVI
Title	:	Crystal Structure of Beta-Lactamase/D-Alanine Carboxypeptidase from Pseudomonas syringae
Authors	:	Kim, Y.; Hatzos-Skintges, C.; Endres, M.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2015-11-19
Resolution	:	1.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

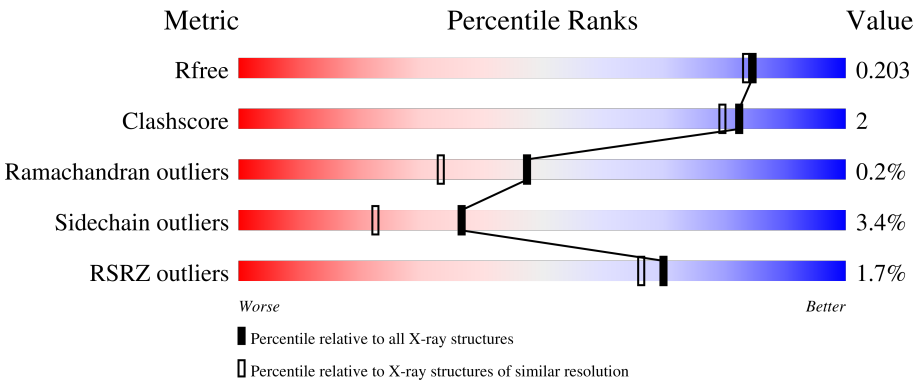
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 of 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 <=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	366	89% 8% • •
2	B	366	87% 11% •
3	C	366	2% 90% 7% • •
4	D	366	4% 91% 7% •

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
5	SO4	A	401	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11790 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-Lactamase/D-Alanine Carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	356	2802	1782	485	527	8	0	4	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP Q87Z37
A	-3	ASN	-	expression tag	UNP Q87Z37
A	-2	ALA	-	expression tag	UNP Q87Z37

- Molecule 2 is a protein called Beta-Lactamase/D-Alanine Carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	359	2804	1784	486	526	8	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	SER	-	expression tag	UNP Q87Z37
B	-3	ASN	-	expression tag	UNP Q87Z37
B	-2	ALA	-	expression tag	UNP Q87Z37

- Molecule 3 is a protein called Beta-Lactamase/D-Alanine Carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
3	C	356	2784	1774	481	521	8	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	SER	-	expression tag	UNP Q87Z37
C	-3	ASN	-	expression tag	UNP Q87Z37
C	-2	ALA	-	expression tag	UNP Q87Z37

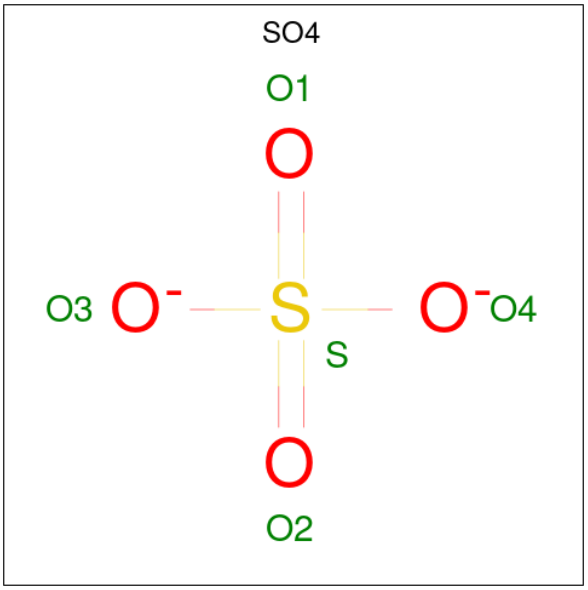
- Molecule 4 is a protein called Beta-Lactamase/D-Alanine Carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
4	D	359	2831	1801	490	532	8	0	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	SER	-	expression tag	UNP Q87Z37
D	-3	ASN	-	expression tag	UNP Q87Z37
D	-2	ALA	-	expression tag	UNP Q87Z37

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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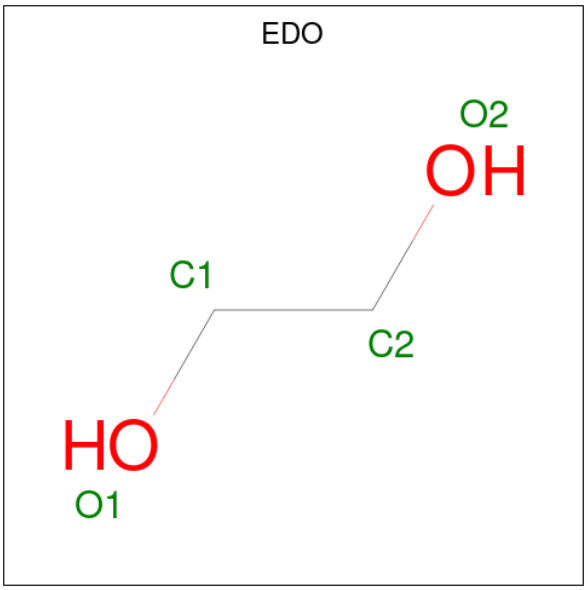
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

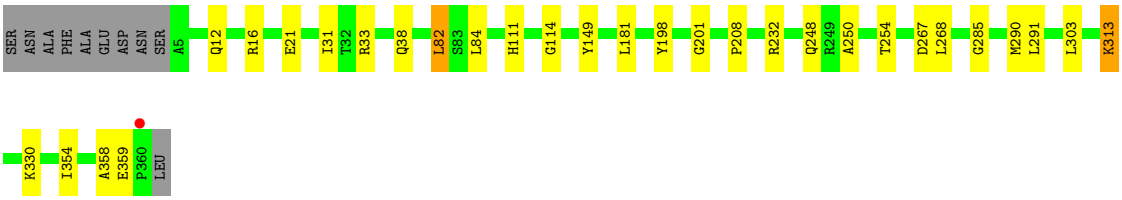
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	139	139	139	0	0
			Total	O		
7	B	157	157	157	0	0
			Total	O		
7	C	97	97	97	0	0
			Total	O		
7	D	117	117	117	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

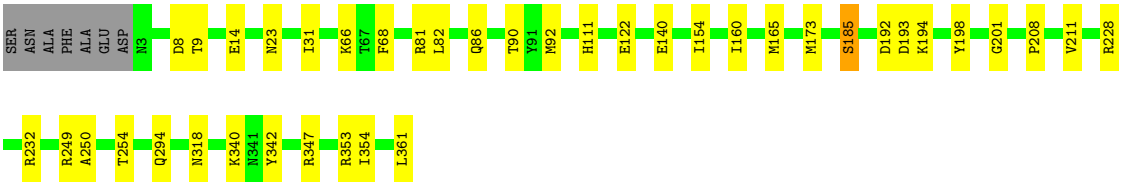
• Molecule 1: Beta-Lactamase/D-Alanine Carboxypeptidase

Chain A:



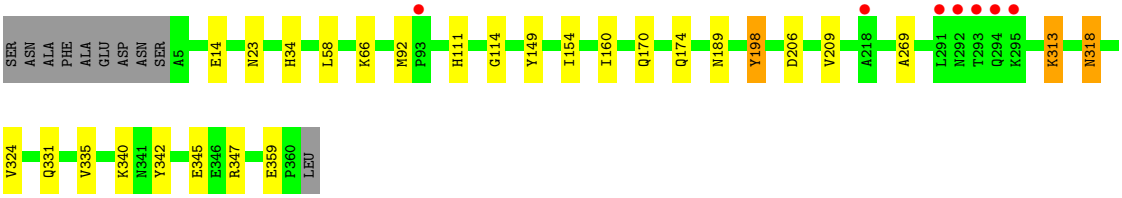
• Molecule 2: Beta-Lactamase/D-Alanine Carboxypeptidase

Chain B:



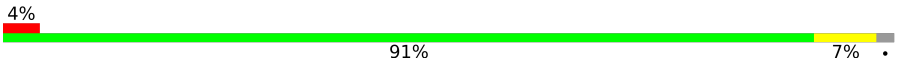
• Molecule 3: Beta-Lactamase/D-Alanine Carboxypeptidase

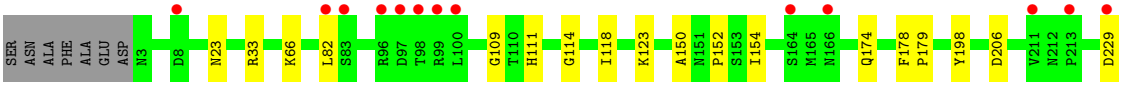
Chain C:

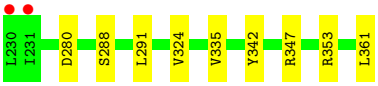


• Molecule 4: Beta-Lactamase/D-Alanine Carboxypeptidase

Chain D:






L230
I231
D280
S288
L291
V324
V335
Y342
R347
R353
L361

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.87Å 72.64Å 93.77Å 89.94° 90.01° 90.08°	Depositor
Resolution (Å)	36.32 – 1.80 36.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (36.32-1.80) 92.8 (36.32-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.163 , 0.201 0.168 , 0.203	Depositor DCC
R_{free} test set	5791 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 20.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.410 for h,-k,-l 0.400 for -h,k,-l 0.439 for -h,-k,l	Xtriage
Reported twinning fraction	0.323 for H, K, L 0.284 for -h,-k,l 0.206 for h,-k,-l 0.187 for -H, K, -L	Depositor
Outliers	0 of 123021 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11790	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MLY, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.61	0/2791	0.78	2/3795 (0.1%)
2	B	0.62	0/2793	0.81	2/3798 (0.1%)
3	C	0.47	0/2773	0.66	0/3771
4	D	0.46	0/2808	0.63	1/3818 (0.0%)
All	All	0.55	0/11165	0.73	5/15182 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	8	ASP	CB-CG-OD1	5.72	123.44	118.30
1	A	267	ASP	CB-CG-OD1	5.47	123.22	118.30
2	B	249	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	303	LEU	CA-CB-CG	5.17	127.19	115.30
4	D	353	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	2802	0	2779	20	0
2	B	2804	0	2791	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2784	0	2773	16	0
4	D	2831	0	2815	10	0
5	A	10	0	0	3	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	4	0	6	0	0
6	B	4	0	6	1	0
6	C	12	0	18	0	0
6	D	4	0	6	0	0
7	A	139	0	0	1	0
7	B	157	0	0	2	0
7	C	97	0	0	1	0
7	D	117	0	0	1	0
All	All	11790	0	11194	56	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 (56) 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:248[B]:GLN:HE21	1:A:248[B]:GLN:HA	1.45	0.82
4:D:324[B]:VAL:HG12	4:D:335:VAL:HG22	1.67	0.74
3:C:269:ALA:HB1	3:C:313:MLY:HH11	1.70	0.73
1:A:33:ARG:HD3	1:A:358:ALA:HB1	1.71	0.72
1:A:313:MLY:CH1	5:A:401:SO4:O2	2.40	0.69
1:A:313:MLY:HH11	5:A:401:SO4:O2	1.95	0.67
3:C:66:LYS:HD2	3:C:313:MLY:CH2	2.28	0.63
1:A:33:ARG:NH1	1:A:358:ALA:O	2.32	0.62
1:A:181:LEU:O	1:A:232:ARG:NH1	2.33	0.62
3:C:170:GLN:OE1	3:C:189:ASN:ND2	2.35	0.60
4:D:111:HIS:HE1	7:D:520:HOH:O	1.84	0.60
3:C:66:LYS:HE3	3:C:154:ILE:HG21	1.86	0.58
3:C:66:LYS:HD2	3:C:313:MLY:HH23	1.88	0.56
2:B:86:GLN:HE21	2:B:90:THR:HG21	1.72	0.55
2:B:111:HIS:HE1	7:B:549:HOH:O	1.90	0.54
3:C:324[B]:VAL:HG12	3:C:335:VAL:HG22	1.91	0.52
4:D:66:LYS:HE3	4:D:154:ILE:HG21	1.91	0.52
1:A:330:MLY:HH13	4:D:361:LEU:CD1	2.40	0.51
2:B:66:LYS:HG2	2:B:154:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:VAL:HG11	3:C:318:ASN:HB3	1.91	0.51
1:A:285:GLY:HA2	1:A:290:MSE:HE3	1.92	0.51
3:C:34:HIS:ND1	3:C:331:GLN:OE1	2.44	0.51
4:D:342:TYR:CZ	4:D:347:ARG:HG2	2.46	0.50
2:B:31:ILE:HD11	2:B:354:ILE:CG2	2.42	0.50
1:A:82:LEU:HD21	1:A:84:LEU:HD23	1.94	0.49
2:B:201:GLY:O	2:B:208:PRO:HA	2.13	0.48
1:A:31:ILE:HD11	1:A:354:ILE:HG21	1.95	0.48
1:A:111:HIS:HE1	7:A:521:HOH:O	1.97	0.48
2:B:250:ALA:O	2:B:254:THR:HG23	2.15	0.47
2:B:342:TYR:CZ	2:B:347:ARG:HG2	2.50	0.46
3:C:66:LYS:CD	3:C:313:MLY:HH21	2.45	0.46
1:A:12:GLN:O	1:A:16:ARG:HG2	2.16	0.46
4:D:178:PHE:HB2	4:D:179:PRO:HD3	1.99	0.45
3:C:342:TYR:CZ	3:C:347:ARG:HG2	2.50	0.45
2:B:185:SER:O	2:B:185:SER:OG	2.32	0.45
1:A:201:GLY:O	1:A:208:PRO:HA	2.17	0.45
2:B:165:MSE:HE2	7:B:651:HOH:O	2.17	0.45
3:C:66:LYS:HD2	3:C:313:MLY:HH21	1.96	0.45
2:B:228:ARG:NH2	6:B:401:EDO:O2	2.50	0.44
4:D:109:GLY:HA2	4:D:154:ILE:HD13	2.00	0.44
1:A:250:ALA:O	1:A:254:THR:HG23	2.18	0.43
3:C:58:LEU:HB2	3:C:198:TYR:HA	2.00	0.43
1:A:330:MLY:HH12	1:A:359:GLU:OE1	2.18	0.43
1:A:149:TYR:OH	1:A:313:MLY:HH11	2.19	0.43
4:D:118:ILE:HD12	4:D:291:LEU:HD22	2.01	0.43
1:A:248[B]:GLN:HA	1:A:248[B]:GLN:NE2	2.24	0.42
1:A:33:ARG:HH21	1:A:38:GLN:NE2	2.17	0.42
1:A:330:MLY:HH13	4:D:361:LEU:HD13	2.00	0.42
2:B:92:MSE:HG2	2:B:160:ILE:HG12	2.01	0.42
2:B:68:PHE:HB3	2:B:173:MSE:HE1	2.01	0.41
1:A:16:ARG:NH1	5:A:400:SO4:O2	2.53	0.41
3:C:92:MSE:HG2	3:C:160:ILE:HG12	2.03	0.41
3:C:111:HIS:HE1	7:C:504:HOH:O	2.03	0.40
3:C:149:TYR:CE1	3:C:313:MLY:HH22	2.56	0.40
4:D:150:ALA:HB1	4:D:152:PRO:HD2	2.02	0.40
3:C:206:ASP:HA	3:C:340:MLY:HH11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/366 (96%)	343 (97%)	8 (2%)	1 (0%)	41	27
2	B	353/366 (96%)	343 (97%)	10 (3%)	0	100	100
3	C	350/366 (96%)	335 (96%)	14 (4%)	1 (0%)	41	27
4	D	355/366 (97%)	342 (96%)	12 (3%)	1 (0%)	41	27
All	All	1410/1464 (96%)	1363 (97%)	44 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	114	GLY
3	C	114	GLY
1	A	114	GLY

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	288/284 (101%)	282 (98%)	6 (2%)	53	42
2	B	289/284 (102%)	271 (94%)	18 (6%)	18	6
3	C	286/284 (101%)	279 (98%)	7 (2%)	49	36
4	D	291/283 (103%)	281 (97%)	10 (3%)	37	22
All	All	1154/1135 (102%)	1113 (96%)	41 (4%)	37	20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21[A]	GLU
1	A	21[B]	GLU
1	A	82	LEU
1	A	198	TYR
1	A	268	LEU
1	A	291	LEU
2	B	9	THR
2	B	14	GLU
2	B	23	ASN
2	B	81	ARG
2	B	82	LEU
2	B	122	GLU
2	B	140	GLU
2	B	185	SER
2	B	192	ASP
2	B	193	ASP
2	B	198	TYR
2	B	211	VAL
2	B	232	ARG
2	B	294	GLN
2	B	318[A]	ASN
2	B	318[B]	ASN
2	B	353	ARG
2	B	361	LEU
3	C	14	GLU
3	C	23	ASN
3	C	174	GLN
3	C	198	TYR
3	C	318	ASN
3	C	345	GLU
3	C	359	GLU
4	D	23	ASN
4	D	33	ARG
4	D	82	LEU
4	D	123	LYS
4	D	174	GLN
4	D	198	TYR
4	D	206	ASP
4	D	229	ASP
4	D	280	ASP
4	D	288	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	38	GLN
1	A	111	HIS
1	A	119	GLN
1	A	125	GLN
1	A	286	ASN
1	A	292	ASN
1	A	294	GLN
1	A	306	GLN
1	A	312	ASN
1	A	356	GLN
1	A	357	HIS
2	B	22	ASN
2	B	23	ASN
2	B	77	GLN
2	B	86	GLN
2	B	111	HIS
2	B	125	GLN
2	B	189	ASN
2	B	292	ASN
2	B	294	GLN
2	B	306	GLN
3	C	20	GLN
3	C	22	ASN
3	C	86	GLN
3	C	111	HIS
3	C	174	GLN
3	C	272	GLN
3	C	286	ASN
3	C	312	ASN
4	D	12	GLN
4	D	22	ASN
4	D	111	HIS
4	D	119	GLN
4	D	125	GLN
4	D	212	ASN
4	D	286	ASN
4	D	292	ASN
4	D	294	GLN
4	D	306	GLN
4	D	312	ASN
4	D	331	GLN
4	D	344	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)

25 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MLY	A	194	1	9,10,11	0.57	0	6,11,13	0.44	0
1	MLY	A	47	1	9,10,11	0.67	0	6,11,13	0.52	0
4	MLY	D	224	4	9,10,11	0.56	0	6,11,13	0.75	0
2	MLY	B	349	2	9,10,11	0.72	0	6,11,13	0.77	0
4	MLY	D	135	4	9,10,11	0.64	0	6,11,13	0.74	0
1	MLY	A	36	1	9,10,11	0.66	0	6,11,13	0.76	0
4	MLY	D	36	4	9,10,11	0.53	0	6,11,13	0.56	0
3	MLY	C	224	3	9,10,11	0.44	0	6,11,13	0.68	0
1	MLY	A	340	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	A	330	1	9,10,11	0.56	0	6,11,13	0.68	0
2	MLY	B	224	2	9,10,11	0.63	0	6,11,13	0.70	0
4	MLY	D	17	4	9,10,11	0.48	0	6,11,13	0.92	0
3	MLY	C	47	3	9,10,11	0.49	0	6,11,13	0.71	0
4	MLY	D	47	4	9,10,11	0.56	0	6,11,13	0.71	0
4	MLY	D	340	4	9,10,11	0.51	0	6,11,13	0.48	0
1	MLY	A	313	1	9,10,11	0.92	0	6,11,13	1.40	1 (16%)
2	MLY	B	36	2	9,10,11	0.70	0	6,11,13	0.66	0
4	MLY	D	330	4	9,10,11	0.60	0	6,11,13	0.63	0
3	MLY	C	330	3	9,10,11	0.56	0	6,11,13	0.39	0
3	MLY	C	36	3	9,10,11	0.58	0	6,11,13	0.41	0
3	MLY	C	340	3	9,10,11	0.64	0	6,11,13	0.43	0
2	MLY	B	194	2	9,10,11	0.59	0	6,11,13	0.87	1 (16%)
2	MLY	B	330	2	9,10,11	0.46	0	6,11,13	0.58	0
2	MLY	B	340	2	9,10,11	0.64	0	6,11,13	0.98	1 (16%)
3	MLY	C	313	3	9,10,11	0.64	0	6,11,13	1.38	1 (16%)

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
1	MLY	A	194	1	-	1/8/9/11	-
1	MLY	A	47	1	-	2/8/9/11	-
4	MLY	D	224	4	-	2/8/9/11	-
2	MLY	B	349	2	-	0/8/9/11	-
4	MLY	D	135	4	-	0/8/9/11	-
1	MLY	A	36	1	-	1/8/9/11	-
4	MLY	D	36	4	-	0/8/9/11	-
3	MLY	C	224	3	-	1/8/9/11	-
1	MLY	A	340	1	-	0/8/9/11	-
1	MLY	A	330	1	-	2/8/9/11	-
2	MLY	B	224	2	-	1/8/9/11	-
4	MLY	D	17	4	-	2/8/9/11	-
3	MLY	C	47	3	-	0/8/9/11	-
4	MLY	D	47	4	-	1/8/9/11	-
4	MLY	D	340	4	-	0/8/9/11	-
1	MLY	A	313	1	-	1/8/9/11	-
2	MLY	B	36	2	-	0/8/9/11	-
4	MLY	D	330	4	-	1/8/9/11	-
3	MLY	C	330	3	-	0/8/9/11	-
3	MLY	C	36	3	-	0/8/9/11	-
3	MLY	C	340	3	-	5/8/9/11	-
2	MLY	B	194	2	-	3/8/9/11	-
2	MLY	B	330	2	-	1/8/9/11	-
2	MLY	B	340	2	-	3/8/9/11	-
3	MLY	C	313	3	-	1/8/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	MLY	CD-CE-NZ	-2.46	107.12	113.79
3	C	313	MLY	CH2-NZ-CE	-2.37	101.33	110.74
2	B	340	MLY	CD-CG-CB	-2.18	105.90	113.62
2	B	194	MLY	CD-CE-NZ	-2.06	108.22	113.79

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	47	MLY	O-C-CA-CB
2	B	194	MLY	C-CA-CB-CG
2	B	340	MLY	O-C-CA-CB
3	C	340	MLY	N-CA-CB-CG
3	C	340	MLY	C-CA-CB-CG
3	C	340	MLY	CD-CE-NZ-CH1
3	C	340	MLY	CD-CE-NZ-CH2
4	D	17	MLY	CD-CE-NZ-CH1
4	D	17	MLY	CD-CE-NZ-CH2
2	B	224	MLY	CG-CD-CE-NZ
1	A	330	MLY	CG-CD-CE-NZ
3	C	313	MLY	CG-CD-CE-NZ
4	D	224	MLY	CG-CD-CE-NZ
2	B	194	MLY	CD-CE-NZ-CH1
2	B	194	MLY	CD-CE-NZ-CH2
4	D	330	MLY	CG-CD-CE-NZ
3	C	340	MLY	CA-CB-CG-CD
4	D	224	MLY	CA-CB-CG-CD
1	A	313	MLY	CE-CD-CG-CB
3	C	224	MLY	CA-CB-CG-CD
1	A	47	MLY	CE-CD-CG-CB
2	B	330	MLY	CG-CD-CE-NZ
4	D	47	MLY	CE-CD-CG-CB
1	A	36	MLY	CG-CD-CE-NZ
2	B	340	MLY	N-CA-CB-CG
1	A	330	MLY	CA-CB-CG-CD
1	A	194	MLY	CD-CE-NZ-CH2
2	B	340	MLY	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	330	MLY	3	0
1	A	313	MLY	3	0
3	C	340	MLY	1	0
3	C	313	MLY	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
5	SO4	C	400	-	4,4,4	0.33	0	6,6,6	0.05	0
5	SO4	B	400	-	4,4,4	0.29	0	6,6,6	0.20	0
5	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.61	0
5	SO4	C	401	-	4,4,4	0.35	0	6,6,6	0.12	0
5	SO4	D	401	-	4,4,4	0.31	0	6,6,6	0.07	0
6	EDO	B	401	-	3,3,3	0.52	0	2,2,2	0.09	0
6	EDO	D	403	-	3,3,3	0.44	0	2,2,2	0.35	0
5	SO4	D	402	-	4,4,4	0.31	0	6,6,6	0.26	0
6	EDO	A	402	-	3,3,3	0.48	0	2,2,2	0.28	0
6	EDO	C	404	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	C	402	-	3,3,3	0.46	0	2,2,2	0.43	0
6	EDO	C	403	-	3,3,3	0.48	0	2,2,2	0.38	0
5	SO4	A	400	-	4,4,4	0.28	0	6,6,6	0.14	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
6	EDO	B	401	-	-	1/1/1/1	-
6	EDO	D	403	-	-	1/1/1/1	-
6	EDO	A	402	-	-	1/1/1/1	-
6	EDO	C	404	-	-	1/1/1/1	-
6	EDO	C	402	-	-	0/1/1/1	-
6	EDO	C	403	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	404	EDO	O1-C1-C2-O2
6	A	402	EDO	O1-C1-C2-O2
6	B	401	EDO	O1-C1-C2-O2
6	D	403	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	SO4	2	0
6	B	401	EDO	1	0
5	A	400	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	342/366 (93%)	-0.40	1 (0%) 94 92	9, 15, 26, 49	0
2	B	345/366 (94%)	-0.42	0 100 100	8, 15, 26, 36	0
3	C	342/366 (93%)	0.08	7 (2%) 65 61	15, 26, 57, 190	0
4	D	344/366 (93%)	0.17	15 (4%) 34 28	17, 29, 62, 120	0
All	All	1373/1464 (93%)	-0.14	23 (1%) 70 66	8, 20, 51, 190	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	293	THR	5.6
3	C	292	ASN	5.1
3	C	294	GLN	5.0
4	D	230	LEU	4.5
4	D	213	PRO	4.3
4	D	96	ARG	4.2
3	C	291	LEU	3.8
4	D	166	ASN	3.3
3	C	218	ALA	2.9
4	D	97	ASP	2.8
3	C	93	PRO	2.7
4	D	99	ARG	2.3
4	D	83	SER	2.2
1	A	360	PRO	2.2
4	D	98	THR	2.1
4	D	229	ASP	2.1
4	D	231	ILE	2.1
3	C	295	LYS	2.1
4	D	100	LEU	2.1
4	D	164[A]	SER	2.1
4	D	8	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	82	LEU	2.0
4	D	211	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
4	MLY	D	17	11/12	0.86	0.15	30,34,37,38	0
4	MLY	D	135	11/12	0.87	0.12	38,40,41,43	0
4	MLY	D	330	11/12	0.89	0.14	35,37,41,42	0
3	MLY	C	36	11/12	0.90	0.12	24,26,30,30	0
1	MLY	A	194	11/12	0.92	0.10	27,31,33,33	0
2	MLY	B	194	11/12	0.93	0.13	23,26,29,29	0
1	MLY	A	330	11/12	0.93	0.11	18,20,26,26	0
3	MLY	C	330	11/12	0.93	0.10	22,23,26,27	0
4	MLY	D	36	11/12	0.94	0.10	29,31,35,35	0
4	MLY	D	47	11/12	0.94	0.10	26,27,28,29	0
3	MLY	C	47	11/12	0.94	0.12	27,28,31,31	0
4	MLY	D	224	11/12	0.94	0.09	21,22,23,23	0
3	MLY	C	313	11/12	0.94	0.13	16,17,21,22	0
2	MLY	B	349	11/12	0.95	0.10	14,15,18,18	0
1	MLY	A	47	11/12	0.95	0.08	17,19,20,20	0
1	MLY	A	36	11/12	0.95	0.10	13,14,15,15	0
3	MLY	C	224	11/12	0.95	0.12	21,24,28,29	0
2	MLY	B	224	11/12	0.95	0.10	12,14,18,18	0
2	MLY	B	330	11/12	0.95	0.09	15,16,18,18	0
1	MLY	A	313	11/12	0.96	0.11	11,12,15,15	0
1	MLY	A	340	11/12	0.96	0.09	12,13,13,13	0
2	MLY	B	36	11/12	0.96	0.08	13,15,17,17	0
2	MLY	B	340	11/12	0.96	0.08	9,10,12,12	0
4	MLY	D	340	11/12	0.96	0.09	24,29,35,35	0
3	MLY	C	340	11/12	0.97	0.07	19,21,24,24	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
6	EDO	D	403	4/4	0.78	0.16	34,35,36,36	0
6	EDO	C	404	4/4	0.88	0.19	31,31,31,32	0
6	EDO	C	402	4/4	0.90	0.11	31,31,31,32	0
6	EDO	A	402	4/4	0.91	0.12	29,29,29,29	0
5	SO4	C	401	5/5	0.91	0.16	52,52,54,55	0
6	EDO	C	403	4/4	0.92	0.12	30,30,30,30	0
5	SO4	D	401	5/5	0.94	0.14	55,56,56,57	0
6	EDO	B	401	4/4	0.95	0.08	17,17,17,18	0
5	SO4	C	400	5/5	0.96	0.09	49,50,51,51	0
5	SO4	A	400	5/5	0.96	0.14	42,43,44,45	0
5	SO4	B	400	5/5	0.96	0.10	38,38,39,39	0
5	SO4	A	401	5/5	0.97	0.08	29,29,31,31	0
5	SO4	D	402	5/5	0.98	0.09	34,34,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.