



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:47 AM UTC

PDB ID : 4MUT / pdb_00004mut
Title : Crystal structure of vancomycin resistance D,D-dipeptidase/D,D-pentapeptidase VanXYc D59S mutant in complex with D-Alanine
Authors : Stogios, P.J.; Evdokimova, E.; Meziane-Cherif, D.; Di Leo, R.; Yim, V.; Courvalin, P.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-09-23
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

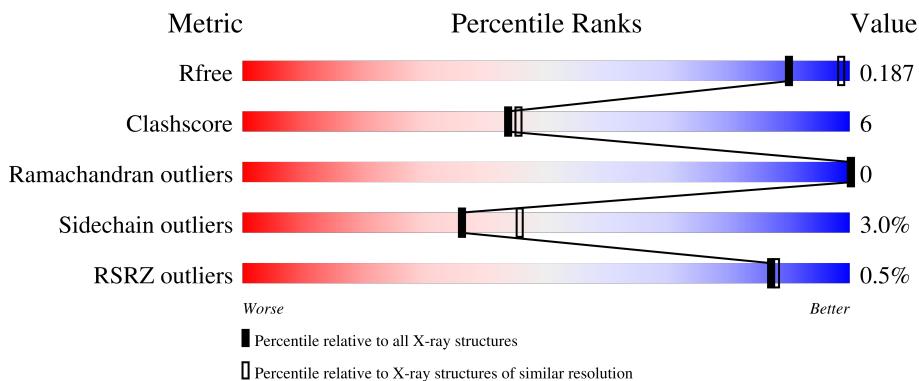
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. 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	211	 76% 10% • 11%
1	B	211	 82% 6% • 11%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3481 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 D,D-dipeptidase/D,D-carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	187	1562	1001	271	285	5	0	1	0
1	B	188	1579	1013	272	289	5	0	3	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q9JN36
A	-19	GLY	-	expression tag	UNP Q9JN36
A	-18	SER	-	expression tag	UNP Q9JN36
A	-17	SER	-	expression tag	UNP Q9JN36
A	-16	HIS	-	expression tag	UNP Q9JN36
A	-15	HIS	-	expression tag	UNP Q9JN36
A	-14	HIS	-	expression tag	UNP Q9JN36
A	-13	HIS	-	expression tag	UNP Q9JN36
A	-12	HIS	-	expression tag	UNP Q9JN36
A	-11	HIS	-	expression tag	UNP Q9JN36
A	-10	SER	-	expression tag	UNP Q9JN36
A	-9	SER	-	expression tag	UNP Q9JN36
A	-8	GLY	-	expression tag	UNP Q9JN36
A	-7	ARG	-	expression tag	UNP Q9JN36
A	-6	GLU	-	expression tag	UNP Q9JN36
A	-5	ASN	-	expression tag	UNP Q9JN36
A	-4	LEU	-	expression tag	UNP Q9JN36
A	-3	TYR	-	expression tag	UNP Q9JN36
A	-2	PHE	-	expression tag	UNP Q9JN36
A	-1	GLN	-	expression tag	UNP Q9JN36
A	0	GLY	-	expression tag	UNP Q9JN36
A	59	SER	ASP	engineered mutation	UNP Q9JN36
B	-20	MET	-	initiating methionine	UNP Q9JN36
B	-19	GLY	-	expression tag	UNP Q9JN36
B	-18	SER	-	expression tag	UNP Q9JN36

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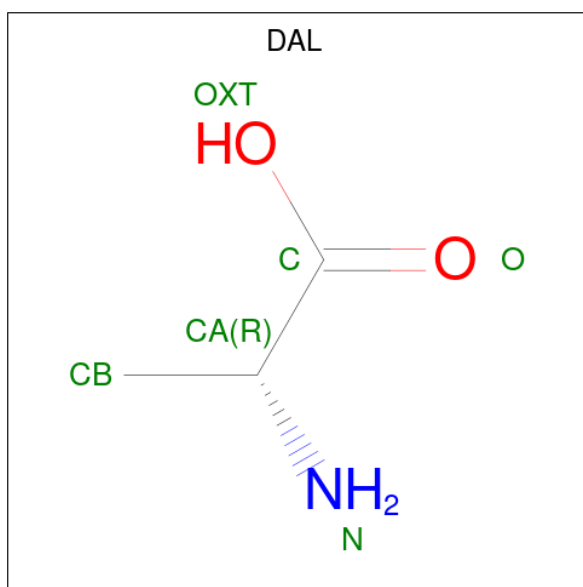
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q9JN36
B	-16	HIS	-	expression tag	UNP Q9JN36
B	-15	HIS	-	expression tag	UNP Q9JN36
B	-14	HIS	-	expression tag	UNP Q9JN36
B	-13	HIS	-	expression tag	UNP Q9JN36
B	-12	HIS	-	expression tag	UNP Q9JN36
B	-11	HIS	-	expression tag	UNP Q9JN36
B	-10	SER	-	expression tag	UNP Q9JN36
B	-9	SER	-	expression tag	UNP Q9JN36
B	-8	GLY	-	expression tag	UNP Q9JN36
B	-7	ARG	-	expression tag	UNP Q9JN36
B	-6	GLU	-	expression tag	UNP Q9JN36
B	-5	ASN	-	expression tag	UNP Q9JN36
B	-4	LEU	-	expression tag	UNP Q9JN36
B	-3	TYR	-	expression tag	UNP Q9JN36
B	-2	PHE	-	expression tag	UNP Q9JN36
B	-1	GLN	-	expression tag	UNP Q9JN36
B	0	GLY	-	expression tag	UNP Q9JN36
B	59	SER	ASP	engineered mutation	UNP Q9JN36

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is D-ALANINE (CCD ID: DAL) (formula: C₃H₇NO₂).

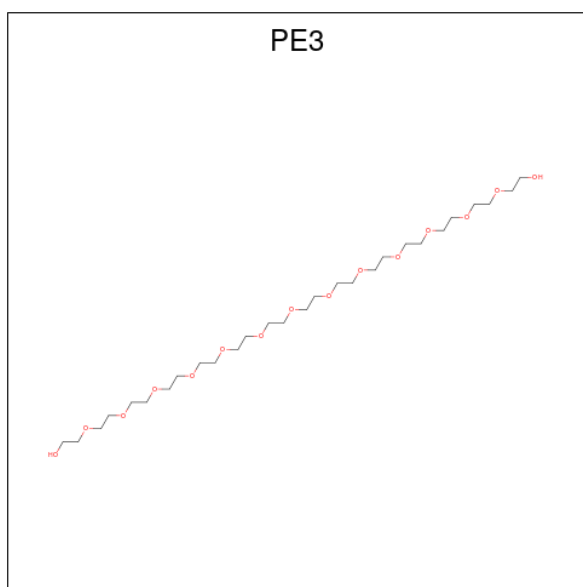


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	6	3	1	2	0	0
3	B	1	6	3	1	2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0

- Molecule 5 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAXAHENTETRACONTANE-1,41-DIOL (CCD ID: PE3) (formula: C₂₈H₅₈O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	170	Total 170	O 170	0	0
7	B	145	Total 145	O 145	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.67Å 45.21Å 63.01Å 86.69° 77.20° 63.88°	Depositor
Resolution (Å)	34.57 – 2.25 34.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.57-2.25) 90.7 (34.57-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.24Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.161 , 0.185 0.163 , 0.187	Depositor DCC
R_{free} test set	1031 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtrriage
Anisotropy	0.602	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3481	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% 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: PE3, ZN, SO4, DAL, 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	0.59	1/1608 (0.1%)	0.89	9/2181 (0.4%)
1	B	0.55	1/1630 (0.1%)	0.87	3/2210 (0.1%)
All	All	0.57	2/3238 (0.1%)	0.88	12/4391 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	TYR	C-O	-5.41	1.17	1.24
1	B	19	PRO	N-CD	5.27	1.55	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	GLN	CA-C-N	-8.54	107.59	123.55
1	B	17	GLN	C-N-CA	-8.54	107.59	123.55
1	A	108	GLN	CA-C-N	8.38	135.04	120.87
1	A	108	GLN	C-N-CA	8.38	135.04	120.87
1	A	106	LYS	CA-C-N	-6.58	112.34	122.60
1	A	106	LYS	C-N-CA	-6.58	112.34	122.60
1	B	142	GLU	N-CA-C	6.52	118.39	111.28
1	A	186	VAL	CA-C-N	-6.50	110.88	122.32
1	A	186	VAL	C-N-CA	-6.50	110.88	122.32
1	A	187	ARG	O-C-N	6.22	131.00	122.41
1	A	12	PRO	CA-C-N	-5.16	112.84	120.94
1	A	12	PRO	C-N-CA	-5.16	112.84	120.94

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	1562	0	1525	29	0
1	B	1579	0	1549	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	6	0	0
3	B	6	0	6	1	0
4	A	1	0	0	0	0
5	A	5	0	4	1	0
6	B	5	0	0	0	0
7	A	170	0	0	0	0
7	B	145	0	0	3	0
All	All	3481	0	3090	38	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 6.

All (38) 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:128:MET:O	1:A:131:MET:HE1	1.63	0.98
1:A:65:LYS:HE2	1:A:68:ARG:NH2	1.83	0.93
1:A:13:LEU:HD21	1:A:97:ILE:CG2	2.00	0.91
1:A:131:MET:HE3	1:A:131:MET:H	1.37	0.89
3:B:202:DAL:N	7:B:444:HOH:O	2.12	0.83
1:A:128:MET:C	1:A:131:MET:HE1	2.04	0.81
1:A:131:MET:HE3	1:A:131:MET:N	1.94	0.81
1:A:65:LYS:HE2	1:A:68:ARG:HH22	1.46	0.79
1:A:127:PHE:O	1:A:131:MET:HE2	1.83	0.78
1:A:6:LEU:HB3	5:A:204:PE3:H382	1.68	0.76
1:A:109:GLU:OE2	1:B:107:LYS:NZ	2.21	0.74
1:A:13:LEU:CD2	1:A:97:ILE:CG2	2.66	0.74
1:A:131:MET:H	1:A:131:MET:CE	2.04	0.70
1:A:13:LEU:HD21	1:A:97:ILE:HG23	1.71	0.69
1:A:13:LEU:HD21	1:A:97:ILE:HG21	1.80	0.64
1:A:184:GLN:HA	1:A:187:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:CE	1:A:68:ARG:NH2	2.63	0.59
1:A:128:MET:C	1:A:131:MET:CE	2.77	0.57
1:B:154:PRO:HD2	1:B:155:TRP:CE3	2.41	0.56
1:A:128:MET:HA	1:A:131:MET:CE	2.38	0.53
1:B:155:TRP:HZ2	7:B:445:HOH:O	1.90	0.52
1:B:18:GLU:H	1:B:18:GLU:CD	2.17	0.52
1:A:109:GLU:O	1:A:110:ASP:C	2.52	0.51
1:B:18:GLU:CD	1:B:18:GLU:N	2.69	0.51
1:A:128:MET:HA	1:A:131:MET:HE2	1.94	0.50
1:A:68:ARG:HA	1:A:90:PRO:HG3	1.93	0.49
1:A:24:LEU:HD21	1:B:113:LEU:HD21	1.95	0.48
1:B:35[B]:GLN:NE2	7:B:330:HOH:O	2.47	0.47
1:B:110:ASP:OD1	1:B:110:ASP:O	2.33	0.47
1:A:14:LYS:NZ	1:A:16:ASN:OD1	2.39	0.46
1:A:145:GLN:HG2	1:A:151:SER:HA	1.98	0.46
1:B:68:ARG:HA	1:B:90:PRO:HG3	1.99	0.45
1:A:65:LYS:HE2	1:A:68:ARG:HH21	1.75	0.44
1:A:109:GLU:CD	1:B:107:LYS:NZ	2.77	0.43
1:A:73:TYR:CD2	1:B:24:LEU:HD23	2.55	0.42
1:B:142:GLU:HA	1:B:152:TYR:HB2	2.01	0.41
1:A:65:LYS:CE	1:A:68:ARG:HH21	2.31	0.41
1:A:128:MET:CA	1:A:131:MET:CE	2.98	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	186/211 (88%)	183 (98%)	3 (2%)	0	100	100
1	B	189/211 (90%)	186 (98%)	3 (2%)	0	100	100
All	All	375/422 (89%)	369 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	168/187 (90%)	162 (96%)	6 (4%)	31	39
1	B	171/187 (91%)	167 (98%)	4 (2%)	44	55
All	All	339/374 (91%)	329 (97%)	10 (3%)	36	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	15	LYS
1	A	17	GLN
1	A	109	GLU
1	A	131	MET
1	A	187	ARG
1	B	18	GLU
1	B	107	LYS
1	B	112	ASP
1	B	131	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	129	GLN
1	B	5	GLN
1	B	11	HIS
1	B	17	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
6	SO4	B	203	-	4,4,4	0.24	0	6,6,6	0.21	0
3	DAL	A	202	-	5,5,5	0.99	0	6,6,6	1.50	2 (33%)
5	PE3	A	204	-	4,4,42	0.72	0	3,3,41	0.40	0
3	DAL	B	202	-	5,5,5	1.38	1 (20%)	6,6,6	0.60	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
3	DAL	A	202	-	-	1/4/4/4	-
5	PE3	A	204	-	-	0/2/2/40	-
3	DAL	B	202	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	DAL	OXT-C	-2.73	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	202	DAL	OXT-C-O	-2.63	118.11	124.08
3	A	202	DAL	OXT-C-CA	2.21	121.41	113.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	DAL	OXT-C-CA-N
3	B	202	DAL	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	204	PE3	1	0
3	B	202	DAL	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	187/211 (88%)	-0.44	1 (0%) 87 88	23, 38, 80, 132	1 (0%)
1	B	188/211 (89%)	-0.39	1 (0%) 87 88	22, 41, 99, 183	3 (1%)
All	All	375/422 (88%)	-0.41	2 (0%) 87 88	22, 40, 95, 183	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	ASP	2.0
1	B	114[A]	ILE	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 oligosaccharides 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
5	PE3	A	204	5/43	0.78	0.14	54,63,65,66	0
4	CL	A	203	1/1	0.94	0.10	64,64,64,64	0
3	DAL	A	202	6/6	0.95	0.11	44,48,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DAL	B	202	6/6	0.96	0.08	31,46,53,64	0
6	SO4	B	203	5/5	0.98	0.05	41,44,53,57	5
2	ZN	B	201	1/1	0.99	0.04	38,38,38,38	1
2	ZN	A	201	1/1	0.99	0.03	29,29,29,29	1

6.5 Other polymers [i](#)

There are no such residues in this entry.