



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 PM UTC

PDB ID : 5C6M / pdb_00005c6m
Title : Crystal structure of deoxyribose-phosphate aldolase from *Shewanella halifaxensis*
Authors : Weiergraeber, O.H.; Dick, M.; Bramski, J.; Pietruszka, J.
Deposited on : 2015-06-23
Resolution : 1.76 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
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

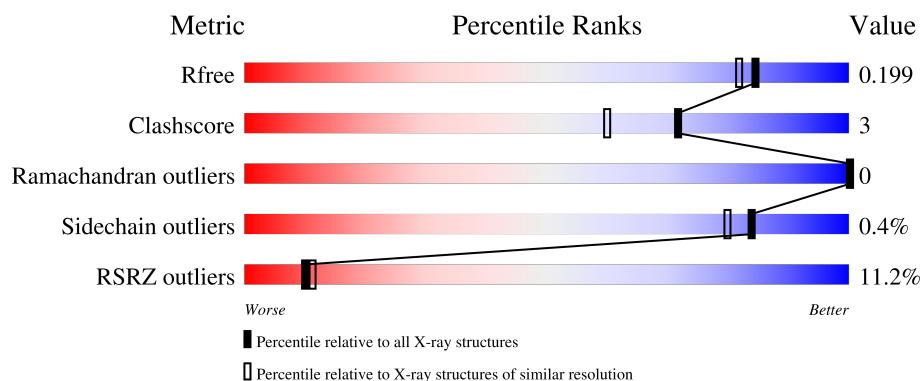
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	265	% 85% 9% 6%
1	B	265	2% 88% 6% 6%
1	C	265	% 86% 6% 7%
1	D	265	38% 83% 11% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8289 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 Deoxyribose-phosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	5	1
			1872	1181	312	370	9			
1	B	248	Total	C	N	O	S	0	9	0
			1896	1195	317	376	8			
1	C	246	Total	C	N	O	S	0	2	0
			1816	1149	298	361	8			
1	D	248	Total	C	N	O	S	0	1	0
			1777	1120	297	352	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	LEU	-	expression tag	UNP B0TQ91
A	259	GLU	-	expression tag	UNP B0TQ91
A	260	HIS	-	expression tag	UNP B0TQ91
A	261	HIS	-	expression tag	UNP B0TQ91
A	262	HIS	-	expression tag	UNP B0TQ91
A	263	HIS	-	expression tag	UNP B0TQ91
A	264	HIS	-	expression tag	UNP B0TQ91
A	265	HIS	-	expression tag	UNP B0TQ91
B	258	LEU	-	expression tag	UNP B0TQ91
B	259	GLU	-	expression tag	UNP B0TQ91
B	260	HIS	-	expression tag	UNP B0TQ91
B	261	HIS	-	expression tag	UNP B0TQ91
B	262	HIS	-	expression tag	UNP B0TQ91
B	263	HIS	-	expression tag	UNP B0TQ91
B	264	HIS	-	expression tag	UNP B0TQ91
B	265	HIS	-	expression tag	UNP B0TQ91
C	258	LEU	-	expression tag	UNP B0TQ91
C	259	GLU	-	expression tag	UNP B0TQ91
C	260	HIS	-	expression tag	UNP B0TQ91
C	261	HIS	-	expression tag	UNP B0TQ91
C	262	HIS	-	expression tag	UNP B0TQ91

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Chain	Residue	Modelled	Actual	Comment	Reference
C	263	HIS	-	expression tag	UNP B0TQ91
C	264	HIS	-	expression tag	UNP B0TQ91
C	265	HIS	-	expression tag	UNP B0TQ91
D	258	LEU	-	expression tag	UNP B0TQ91
D	259	GLU	-	expression tag	UNP B0TQ91
D	260	HIS	-	expression tag	UNP B0TQ91
D	261	HIS	-	expression tag	UNP B0TQ91
D	262	HIS	-	expression tag	UNP B0TQ91
D	263	HIS	-	expression tag	UNP B0TQ91
D	264	HIS	-	expression tag	UNP B0TQ91
D	265	HIS	-	expression tag	UNP B0TQ91

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	324	Total O 324 324	0	0
4	B	308	Total O 308 308	0	0
4	C	189	Total O 189 189	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	101	Total 101	O 101	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.03Å 52.51Å 143.21Å 90.00° 122.34° 90.00°	Depositor
Resolution (Å)	48.70 – 1.76 48.70 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.70-1.76) 99.5 (48.70-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.168 , 0.198 0.170 , 0.199	Depositor DCC
R_{free} test set	4796 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8289	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: NA, 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	0.44	0/1897	0.74	0/2574
1	B	0.46	0/1921	0.74	0/2607
1	C	0.36	0/1841	0.74	0/2507
1	D	0.37	0/1802	0.77	2/2455 (0.1%)
All	All	0.41	0/7461	0.75	2/10143 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ALA	N-CA-C	6.26	117.91	111.14
1	D	174	VAL	N-CA-C	-5.02	99.90	107.73

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	1872	0	1889	14	0
1	B	1896	0	1912	9	0
1	C	1816	0	1801	9	0
1	D	1777	0	1723	16	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	324	0	0	4	0
4	B	308	0	0	4	0
4	C	189	0	0	0	0
4	D	101	0	0	0	0
All	All	8289	0	7325	48	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 3.

All (48) 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:9:GLN:NE2	4:A:401:HOH:O	2.21	0.73
1:B:108[B]:ARG:NH1	4:B:402:HOH:O	2.21	0.73
1:A:108[B]:ARG:NH1	4:A:404:HOH:O	2.23	0.71
1:C:19:THR:HG22	1:C:32:LEU:HD22	1.78	0.66
1:A:19:THR:HG22	1:A:32:LEU:HD22	1.82	0.61
1:B:27[B]:GLN:NE2	4:B:404:HOH:O	2.24	0.61
1:C:234:ALA:HB1	1:C:237:LEU:HB3	1.87	0.56
1:D:144:LEU:O	1:D:146:ASP:N	2.41	0.53
1:C:166:LYS:HD2	1:C:198:LYS:HD3	1.91	0.53
1:D:138:ILE:HG12	1:D:166:LYS:HD3	1.91	0.52
1:D:19:THR:HG22	1:D:32:LEU:HD22	1.92	0.52
1:B:19:THR:HG22	1:B:32:LEU:HD22	1.91	0.52
1:D:111:MET:HE2	1:D:144:LEU:HA	1.91	0.51
1:A:1:MET:HB3	1:A:4:LEU:HB2	1.93	0.51
1:D:129:CYS:HB3	1:D:133:THR:O	2.11	0.50
1:C:35:LYS:HE2	1:C:238:LEU:HD23	1.94	0.50
1:D:136:LYS:HG2	1:D:164:PHE:HB2	1.92	0.50
1:D:234:ALA:HB1	1:D:237:LEU:HB3	1.94	0.50
1:C:199:PRO:HD2	1:C:231:ARG:O	2.12	0.49
1:D:159:ASP:OD1	1:D:191:LYS:NZ	2.45	0.49
1:C:17:LEU:HG	1:C:32:LEU:HD11	1.96	0.47
1:A:100:GLU:HG2	1:A:134:ILE:HG12	1.97	0.47
1:B:100:GLU:HG2	1:B:134:ILE:HB	1.96	0.47
1:A:108[B]:ARG:NH1	4:A:412:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ALA:HB2	1:C:69:LYS:HB2	1.97	0.46
1:A:115:GLU:CD	1:A:152:LYS:HE2	2.41	0.46
1:D:166:LYS:HD2	1:D:198:LYS:HD3	1.96	0.46
1:B:199:PRO:HD2	1:B:231:ARG:O	2.16	0.46
1:D:87:VAL:HG12	1:D:91:ARG:HD2	1.98	0.46
1:A:199:PRO:HD2	1:A:231:ARG:O	2.15	0.46
1:B:1:MET:O	1:B:5:LYS:N	2.38	0.45
1:D:17:LEU:HG	1:D:32:LEU:HD11	1.98	0.45
1:B:146:ASP:OD1	4:B:403:HOH:O	2.21	0.45
1:A:1:MET:O	1:A:5:LYS:N	2.39	0.45
1:B:9:GLN:NE2	4:B:401:HOH:O	2.20	0.44
1:D:199:PRO:HD2	1:D:231:ARG:O	2.18	0.43
1:C:136:LYS:HG2	1:C:164:PHE:HB2	1.98	0.43
1:A:239:THR:HG22	1:A:243:HIS:CE1	2.54	0.43
1:A:136:LYS:HG2	1:A:164:PHE:HB2	2.02	0.42
1:C:179:GLU:H	1:C:179:GLU:CD	2.28	0.42
1:A:179:GLU:HG3	4:A:582:HOH:O	2.20	0.41
1:D:100:GLU:HG2	1:D:134:ILE:HG12	2.02	0.41
1:D:248:ALA:O	1:D:249:ASP:HB2	2.20	0.41
1:D:197:PHE:CE2	1:D:199:PRO:HD3	2.56	0.41
1:B:239[A]:THR:HG22	1:B:243:HIS:CE1	2.55	0.41
1:A:182:GLU:CD	1:A:218:ARG:HH22	2.29	0.41
1:A:35:LYS:HE3	1:A:238:LEU:HD23	2.03	0.40
1:D:166:LYS:HE2	1:D:168:SER:O	2.21	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	251/265 (95%)	243 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	255/265 (96%)	247 (97%)	8 (3%)	0	100	100
1	C	246/265 (93%)	241 (98%)	5 (2%)	0	100	100
1	D	247/265 (93%)	237 (96%)	10 (4%)	0	100	100
All	All	999/1060 (94%)	968 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	195/205 (95%)	194 (100%)	1 (0%)	81	75
1	B	197/205 (96%)	196 (100%)	1 (0%)	81	75
1	C	184/205 (90%)	183 (100%)	1 (0%)	81	75
1	D	173/205 (84%)	173 (100%)	0	100	100
All	All	749/820 (91%)	746 (100%)	3 (0%)	84	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	B	38	THR
1	C	38	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	61	ASN
1	B	21	ASN
1	B	243	HIS
1	C	21	ASN

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Mol	Chain	Res	Type
1	D	61	ASN
1	D	243	HIS

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	248/265 (93%)	-0.38	3 (1%) 76 82	11, 23, 40, 72	5 (2%)
1	B	248/265 (93%)	-0.38	5 (2%) 65 71	10, 24, 39, 73	9 (3%)
1	C	246/265 (92%)	0.13	2 (0%) 82 86	16, 37, 65, 87	2 (0%)
1	D	248/265 (93%)	1.83	101 (40%) 0 1	34, 66, 91, 111	1 (0%)
All	All	990/1060 (93%)	0.30	111 (11%) 10 11	10, 32, 83, 111	17 (1%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	ALA	5.4
1	D	176	ALA	4.6
1	D	158	ILE	4.5
1	D	174	VAL	4.5
1	D	79	GLY	4.4
1	D	172	VAL	4.4
1	B	1	MET	4.4
1	D	160	ALA	4.3
1	D	219	LEU	4.2
1	D	110	LEU	4.2
1	D	193	PRO	4.0
1	D	187	VAL	4.0
1	C	247	LEU	3.9
1	D	122	VAL	3.9
1	B	247	LEU	3.9
1	D	144	LEU	3.9
1	B	248	ALA	3.8
1	D	119	PHE	3.7
1	D	145	ALA	3.7
1	D	156	LEU	3.5
1	A	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	149	LEU	3.5
1	D	107	TYR	3.5
1	D	225	ALA	3.5
1	D	150	ILE	3.4
1	D	154	SER	3.4
1	D	164	PHE	3.4
1	D	117	VAL	3.4
1	D	165	ILE	3.4
1	D	116	THR	3.3
1	D	248	ALA	3.3
1	D	183	ILE	3.3
1	D	128	ALA	3.3
1	D	78	HIS	3.3
1	D	84	ALA	3.3
1	D	195	VAL	3.2
1	D	109	ALA	3.2
1	D	162	ALA	3.2
1	D	3	ASP	3.2
1	D	143	VAL	3.2
1	D	105	PHE	3.1
1	D	135	LEU	3.1
1	D	194	LYS	3.1
1	D	134	ILE	3.1
1	D	139	ILE	3.1
1	D	14	LEU	3.1
1	D	137	VAL	3.0
1	D	83	ILE	3.0
1	D	216	ALA	3.0
1	D	228	ALA	3.0
1	D	224	TRP	3.0
1	D	153	ALA	3.0
1	D	178	LEU	3.0
1	D	188	ILE	3.0
1	A	202	GLY	3.0
1	D	77	PRO	3.0
1	D	215	VAL	2.9
1	D	7	ALA	2.9
1	B	202[A]	GLY	2.9
1	D	197	PHE	2.8
1	D	209	ALA	2.8
1	D	111	MET	2.8
1	D	173	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	104	VAL	2.8
1	D	4	LEU	2.8
1	D	81	ASP	2.8
1	D	141	SER	2.8
1	D	189	SER	2.8
1	D	177	THR	2.7
1	D	180	ALA	2.7
1	D	121	LEU	2.7
1	D	22	ASP	2.7
1	A	2	SER	2.6
1	D	220	LEU	2.6
1	D	86	ALA	2.6
1	D	175	ASN	2.5
1	D	191	LYS	2.5
1	D	192	ASN	2.4
1	D	230	PHE	2.4
1	D	186	THR	2.4
1	D	103	VAL	2.4
1	D	159	ASP	2.4
1	D	179	GLU	2.4
1	D	87	VAL	2.3
1	D	212	PHE	2.3
1	D	68	ILE	2.3
1	D	75	ASN	2.3
1	D	168	SER	2.3
1	C	2	SER	2.3
1	D	2	SER	2.3
1	D	76	PHE	2.3
1	B	2	SER	2.2
1	D	152	LYS	2.2
1	D	131	GLU	2.2
1	D	138	ILE	2.2
1	D	147	PRO	2.2
1	D	157	SER	2.2
1	D	113	GLY	2.2
1	D	223	ASP	2.1
1	D	124	ALA	2.1
1	D	196	GLY	2.1
1	D	181	ALA	2.1
1	D	106	PRO	2.1
1	D	85	ILE	2.1
1	D	201	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	127	GLU	2.1
1	D	206	ALA	2.0
1	D	184	MET	2.0
1	D	161	GLY	2.0
1	D	217	ALA	2.0
1	D	125	CYS	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($\text{\AA}^2$)	Q<0.9
3	CL	D	301	1/1	0.94	0.18	41,41,41,41	0
2	NA	A	301	1/1	0.95	0.09	35,35,35,35	0
3	CL	C	301	1/1	0.96	0.10	43,43,43,43	0
2	NA	B	301	1/1	0.96	0.06	35,35,35,35	0
3	CL	A	302	1/1	0.99	0.08	23,23,23,23	0
3	CL	B	302	1/1	0.99	0.09	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.