Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 07:47 PM EDT

PDB ID	:	9NF3 / pdb_00009nf3
Title	:	cis-CaaD E114D mutant with a covalent ethylene intermediate of the hydration and decarboxylation of cis-3-chloroacrylic acid
Authors	:	Silva, K.; Geiger, J.H.; Draths, K.
Deposited on	:	2025-02-20
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 ⓘ 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:

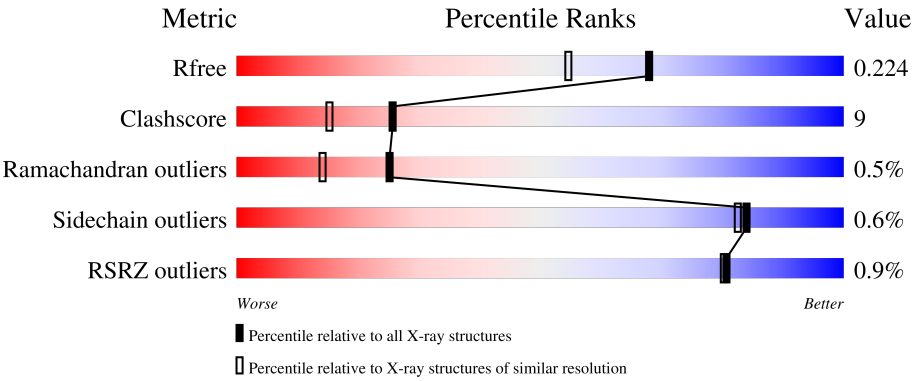
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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	164	% 75% 12% • 12%
1	B	164	% 72% 16% • 12%
2	C	164	% 76% 13% 11%

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	SO4	C	201	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3864 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 Cis-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	145	Total	C	N	O	S	0	1	0
			1152	723	209	216	4			
1	A	145	Total	C	N	O	S	0	0	0
			1141	717	205	215	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	ASP	GLU	engineered mutation	UNP Q6VPE5
B	150	GLU	-	expression tag	UNP Q6VPE5
B	151	ASN	-	expression tag	UNP Q6VPE5
B	152	LEU	-	expression tag	UNP Q6VPE5
B	153	TYR	-	expression tag	UNP Q6VPE5
B	154	PHE	-	expression tag	UNP Q6VPE5
B	155	GLN	-	expression tag	UNP Q6VPE5
B	156	GLY	-	expression tag	UNP Q6VPE5
B	157	LEU	-	expression tag	UNP Q6VPE5
B	158	GLU	-	expression tag	UNP Q6VPE5
B	159	HIS	-	expression tag	UNP Q6VPE5
B	160	HIS	-	expression tag	UNP Q6VPE5
B	161	HIS	-	expression tag	UNP Q6VPE5
B	162	HIS	-	expression tag	UNP Q6VPE5
B	163	HIS	-	expression tag	UNP Q6VPE5
B	164	HIS	-	expression tag	UNP Q6VPE5
A	114	ASP	GLU	engineered mutation	UNP Q6VPE5
A	150	GLU	-	expression tag	UNP Q6VPE5
A	151	ASN	-	expression tag	UNP Q6VPE5
A	152	LEU	-	expression tag	UNP Q6VPE5
A	153	TYR	-	expression tag	UNP Q6VPE5
A	154	PHE	-	expression tag	UNP Q6VPE5
A	155	GLN	-	expression tag	UNP Q6VPE5
A	156	GLY	-	expression tag	UNP Q6VPE5
A	157	LEU	-	expression tag	UNP Q6VPE5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLU	-	expression tag	UNP Q6VPE5
A	159	HIS	-	expression tag	UNP Q6VPE5
A	160	HIS	-	expression tag	UNP Q6VPE5
A	161	HIS	-	expression tag	UNP Q6VPE5
A	162	HIS	-	expression tag	UNP Q6VPE5
A	163	HIS	-	expression tag	UNP Q6VPE5
A	164	HIS	-	expression tag	UNP Q6VPE5

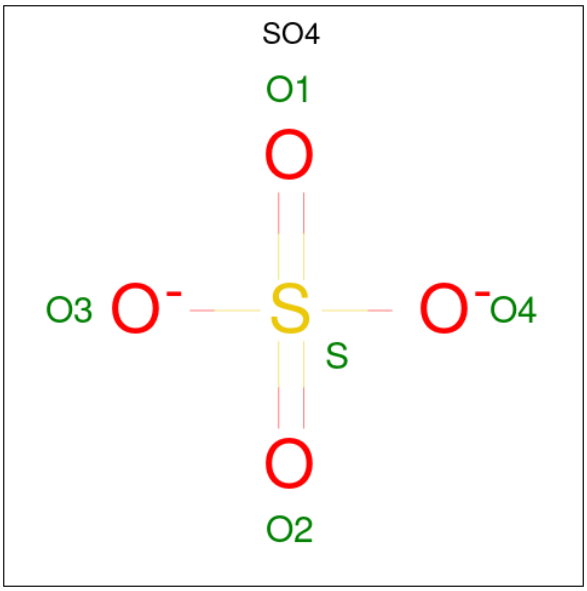
- Molecule 2 is a protein called Cis-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	146	Total	C	N	O	S	0	0	0
			1150	724	206	216	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	114	ASP	GLU	engineered mutation	UNP Q6VPE5
C	150	GLU	-	expression tag	UNP Q6VPE5
C	151	ASN	-	expression tag	UNP Q6VPE5
C	152	LEU	-	expression tag	UNP Q6VPE5
C	153	TYR	-	expression tag	UNP Q6VPE5
C	154	PHE	-	expression tag	UNP Q6VPE5
C	155	GLN	-	expression tag	UNP Q6VPE5
C	156	GLY	-	expression tag	UNP Q6VPE5
C	157	LEU	-	expression tag	UNP Q6VPE5
C	158	GLU	-	expression tag	UNP Q6VPE5
C	159	HIS	-	expression tag	UNP Q6VPE5
C	160	HIS	-	expression tag	UNP Q6VPE5
C	161	HIS	-	expression tag	UNP Q6VPE5
C	162	HIS	-	expression tag	UNP Q6VPE5
C	163	HIS	-	expression tag	UNP Q6VPE5
C	164	HIS	-	expression tag	UNP Q6VPE5

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

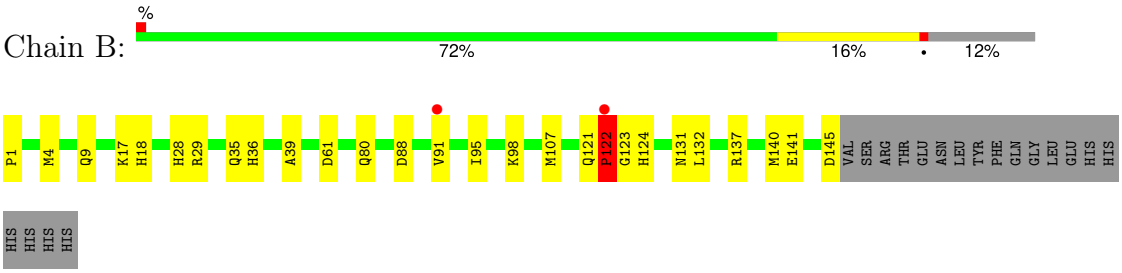
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	146	Total O 146 146	0	0
4	C	152	Total O 152 152	0	0
4	A	108	Total O 108 108	0	0

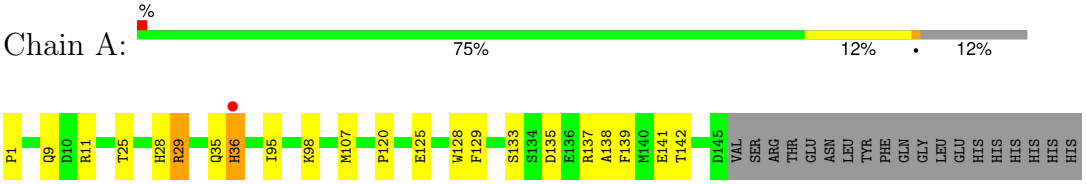
3 Residue-property plots (i)

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.

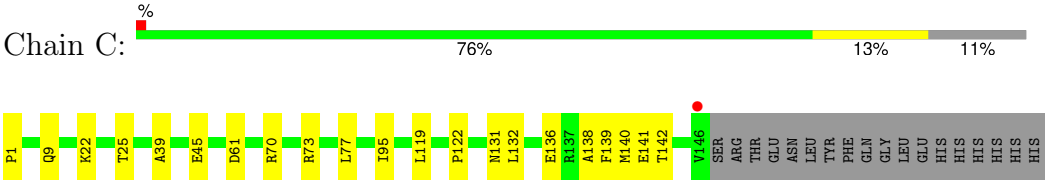
• Molecule 1: Cis-3-chloroacrylic acid dehalogenase



• Molecule 1: Cis-3-chloroacrylic acid dehalogenase



• Molecule 2: Cis-3-chloroacrylic acid dehalogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	59.53Å 99.94Å 142.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 1.80 29.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.7 (29.77-1.80) 90.6 (29.77-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.180 , 0.224 0.180 , 0.224	Depositor DCC
R_{free} test set	37725 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.058 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3864	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N80, 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	0.29	0/1169	0.54	1/1583 (0.1%)
1	B	0.32	0/1180	0.57	0/1597
2	C	0.33	0/1168	0.55	0/1582
All	All	0.31	0/3517	0.55	1/4762 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	ARG	CB-CG-CD	5.75	124.51	111.30

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	1141	0	1084	21	0
1	B	1152	0	1096	25	0
2	C	1150	0	1094	19	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	3	0
4	A	108	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	146	0	0	6	3
4	C	152	0	0	5	2
All	All	3864	0	3274	63	3

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 9.

All (63) 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)
2:C:73:ARG:NH1	3:C:201:SO4:O1	1.95	0.98
1:B:29[B]:ARG:NH1	4:B:301:HOH:O	1.94	0.97
2:C:131:ASN:ND2	4:C:301:HOH:O	2.01	0.93
2:C:70:ARG:HD2	2:C:119:LEU:HD13	1.53	0.90
1:B:122:PRO:O	1:B:124:HIS:N	2.16	0.78
2:C:70:ARG:HD3	3:C:201:SO4:O2	1.82	0.77
1:A:135:ASP:OD2	4:A:302:HOH:O	2.05	0.74
2:C:61:ASP:O	2:C:95:ILE:HD11	1.89	0.71
2:C:61:ASP:OD2	4:C:302:HOH:O	2.09	0.71
1:B:80:GLN:OE1	4:B:302:HOH:O	2.08	0.70
1:A:1:PRO:HG3	1:A:28:HIS:CE1	2.30	0.66
1:B:98:LYS:HE2	1:A:139:PHE:CD1	2.32	0.65
1:A:141:GLU:OE1	4:A:303:HOH:O	2.14	0.64
1:A:137:ARG:O	1:A:141:GLU:HG3	1.98	0.64
1:B:137:ARG:O	1:B:141:GLU:HG3	1.98	0.63
2:C:9:GLN:HG3	2:C:45:GLU:HB3	1.83	0.60
1:A:29:ARG:NH1	4:A:301:HOH:O	2.00	0.57
2:C:1:N80:H2	3:C:201:SO4:O3	2.06	0.55
1:A:129:PHE:CZ	1:A:137:ARG:HB3	2.41	0.55
2:C:73:ARG:HD3	2:C:77:LEU:HD23	1.89	0.54
1:B:1:PRO:HG3	1:B:28:HIS:CD2	2.42	0.54
1:B:9:GLN:OE1	4:B:303:HOH:O	2.19	0.53
1:A:1:PRO:HG3	1:A:28:HIS:NE2	2.23	0.53
1:A:133:SER:O	1:A:137:ARG:HG3	2.09	0.53
1:A:138:ALA:O	1:A:142:THR:HG23	2.09	0.52
1:B:88:ASP:HA	1:B:91:VAL:HG22	1.91	0.52
1:B:132:LEU:HD13	1:B:140:MET:HE1	1.91	0.51
2:C:22:LYS:HB2	4:C:409:HOH:O	2.11	0.50
1:B:61:ASP:O	1:B:95:ILE:HD11	2.12	0.49
1:B:1:PRO:HG3	1:B:28:HIS:CE1	2.48	0.49
1:B:1:PRO:HD2	1:B:39:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HE	1:A:95:ILE:HD11	1.78	0.47
1:B:122:PRO:C	1:B:124:HIS:H	2.18	0.47
2:C:61:ASP:HB2	4:C:401:HOH:O	2.14	0.47
2:C:25:THR:HG23	2:C:39:ALA:HB3	1.97	0.47
1:B:29[B]:ARG:NH1	1:B:36:HIS:H	2.13	0.46
1:A:120:PRO:HG3	1:A:128:TRP:CB	2.46	0.46
1:B:17:LYS:NZ	4:B:306:HOH:O	2.36	0.46
1:A:11:ARG:HH21	1:A:95:ILE:HG12	1.79	0.46
1:A:29:ARG:NH2	1:A:36:HIS:CG	2.83	0.46
1:A:1:PRO:HG3	1:A:28:HIS:CD2	2.52	0.45
1:B:29[B]:ARG:NH1	1:B:35:GLN:HA	2.31	0.45
1:A:25:THR:HG22	1:A:36:HIS:CD2	2.52	0.45
1:B:1:PRO:HG3	1:B:28:HIS:NE2	2.32	0.45
2:C:70:ARG:NH2	2:C:122:PRO:HA	2.32	0.45
1:A:9:GLN:NE2	4:A:304:HOH:O	2.25	0.45
2:C:136:GLU:O	2:C:140:MET:HG3	2.17	0.44
2:C:132:LEU:HD13	2:C:140:MET:CE	2.48	0.44
2:C:141:GLU:OE1	4:C:303:HOH:O	2.21	0.44
2:C:132:LEU:HD13	2:C:140:MET:HE1	2.00	0.43
2:C:138:ALA:O	2:C:142:THR:HG23	2.18	0.43
1:B:29[A]:ARG:HE	1:B:29[A]:ARG:HB3	1.50	0.43
1:A:107:MET:HE3	1:A:107:MET:HB2	1.89	0.43
1:B:29[B]:ARG:NH1	4:B:309:HOH:O	2.50	0.43
2:C:139:PHE:CE1	1:A:98:LYS:HE3	2.53	0.43
1:B:121:GLN:O	1:B:122:PRO:O	2.37	0.42
1:B:131:ASN:HB3	4:B:411:HOH:O	2.19	0.42
1:B:29[B]:ARG:CZ	1:B:35:GLN:HA	2.49	0.42
1:B:4:MET:HE3	1:B:4:MET:HB3	1.92	0.42
1:B:18:HIS:NE2	1:B:145:ASP:OD2	2.43	0.42
1:B:107:MET:HE3	1:B:107:MET:HB2	1.72	0.42
1:A:29:ARG:NH2	1:A:36:HIS:HB2	2.34	0.42
1:A:35:GLN:OE1	1:A:125:GLU:HB3	2.21	0.40

All (3) 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)
4:B:437:HOH:O	4:C:413:HOH:O[3_554]	1.93	0.27
4:B:343:HOH:O	4:B:429:HOH:O[3_554]	2.03	0.17
4:B:404:HOH:O	4:C:413:HOH:O[3_554]	2.19	0.01

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	143/164 (87%)	141 (99%)	2 (1%)	0	100 100
1	B	144/164 (88%)	140 (97%)	2 (1%)	2 (1%)	9 2
2	C	144/164 (88%)	143 (99%)	1 (1%)	0	100 100
All	All	431/492 (88%)	424 (98%)	5 (1%)	2 (0%)	25 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	PRO
1	B	123	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	118/136 (87%)	117 (99%)	1 (1%)	79 76
1	B	119/136 (88%)	118 (99%)	1 (1%)	79 76
2	C	118/135 (87%)	118 (100%)	0	100 100
All	All	355/407 (87%)	353 (99%)	2 (1%)	84 82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	PRO

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Mol	Chain	Res	Type
1	A	36	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	ASN
2	C	9	GLN
2	C	110	GLN
1	A	18	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)

1 non-standard protein/DNA/RNA residue is 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	N80	C	1	2	8,9,10	0.81	0	5,11,13	1.22	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	N80	C	1	2	-	0/0/14/16	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	N80	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	SO4	C	201	-	4,4,4	0.26	0	6,6,6	0.64	0
3	SO4	B	201	-	4,4,4	0.86	0	6,6,6	0.67	0
3	SO4	A	201	-	4,4,4	0.21	0	6,6,6	0.45	0

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	SO4	3	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, 95^{th} 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	145/164 (88%)	-0.06	1 (0%)	84	84	18, 27, 41, 50	0
1	B	145/164 (88%)	-0.24	2 (1%)	73	72	14, 25, 33, 42	1 (0%)
2	C	145/164 (88%)	-0.22	1 (0%)	84	84	17, 23, 36, 48	0
All	All	435/492 (88%)	-0.18	4 (0%)	81	80	14, 25, 39, 50	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	146	VAL	3.0
1	A	36	HIS	2.5
1	B	91	VAL	2.2
1	B	122	PRO	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	N80	C	1	9/10	0.95	0.08	19,26,28,29	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
3	SO4	C	201	5/5	0.91	0.11	29,31,32,39	0
3	SO4	B	201	5/5	0.92	0.10	23,27,31,33	0
3	SO4	A	201	5/5	0.95	0.08	27,30,36,38	0

6.5 Other polymers

There are no such residues in this entry.