Full wwPDB X-ray Structure Validation Report (i)

Mar 25, 2025 – 08:09 AM EDT

PDB ID	:	9NF9
Title	:	cis-CaaD E114N mutant apo
Authors	:	Silva, K.; Geiger, J.H.; Draths, K.
Deposited on	:	2025-02-21
Resolution	:	2.51 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 (1)) were used in the production of this report:

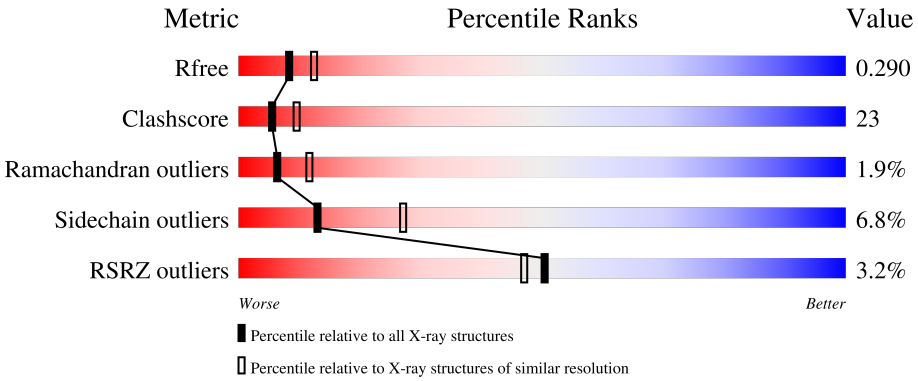
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.51 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	165	2% 62% 24% • 12%
1	B	165	5% 47% 33% 7% • 12%
1	C	165	% 50% 32% • • 12%

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
2	SO4	A	201	-	-	X	-
2	SO4	B	201	-	-	X	-
2	SO4	C	201	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3490 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	A	145	Total	C	N	O	S	0	0	0
			1141	717	206	214	4			
1	B	145	Total	C	N	O	S	0	0	0
			1136	714	204	214	4			
1	C	145	Total	C	N	O	S	0	0	0
			1141	717	206	214	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ASN	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
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
B	114	ASN	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

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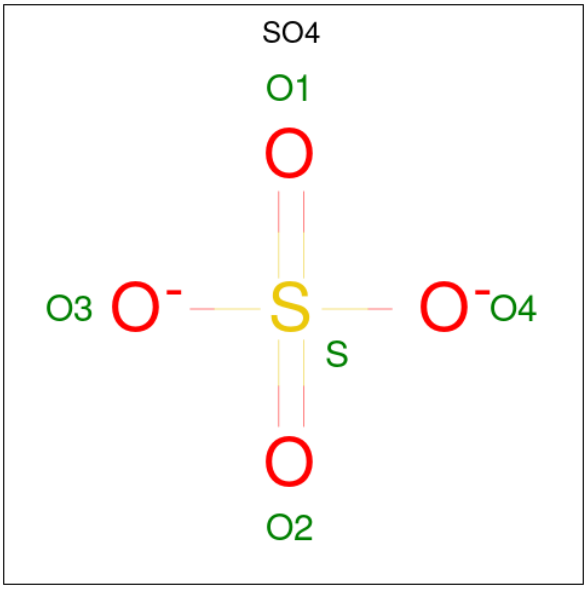
Chain	Residue	Modelled	Actual	Comment	Reference
B	156	GLY	-	expression tag	UNP Q6VPE5
B	157	LEU	-	expression tag	UNP Q6VPE5
B	158	GLU	-	expression tag	UNP Q6VPE5
B	159	HIS	-	expression tag	UNP Q6VPE5
B	160	HIS	-	expression tag	UNP Q6VPE5
B	161	HIS	-	expression tag	UNP Q6VPE5
B	162	HIS	-	expression tag	UNP Q6VPE5
B	163	HIS	-	expression tag	UNP Q6VPE5
B	164	HIS	-	expression tag	UNP Q6VPE5
C	114	ASN	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 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

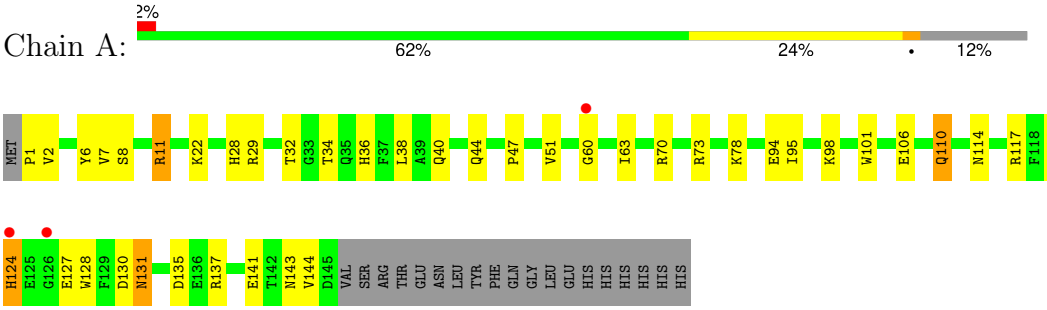
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	21	Total O 21 21	0	0
3	C	17	Total O 17 17	0	0

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.

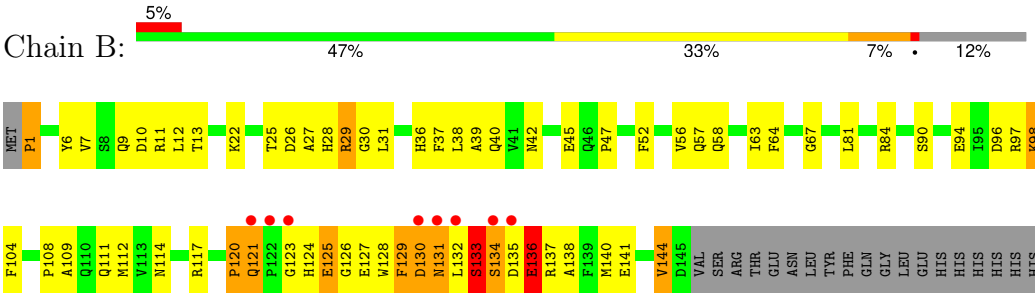
• Molecule 1: Cis-3-chloroacrylic acid dehalogenase

Chain A:



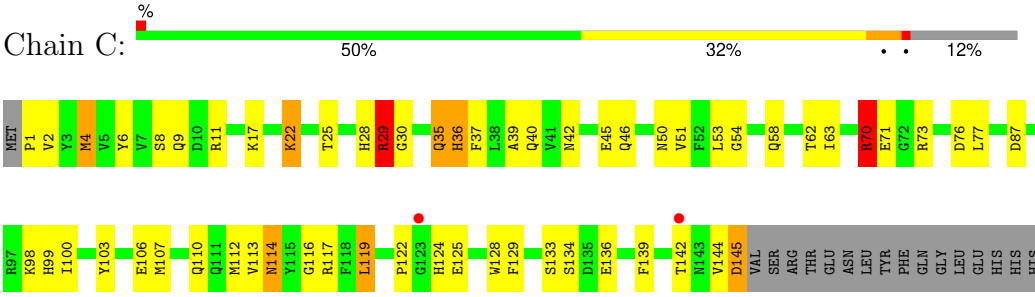
• Molecule 1: Cis-3-chloroacrylic acid dehalogenase

Chain B:



• Molecule 1: Cis-3-chloroacrylic acid dehalogenase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	58.22Å 99.02Å 137.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 2.51 28.71 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.2 (28.71-2.51) 89.1 (28.71-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.215 , 0.290 0.215 , 0.290	Depositor DCC
R_{free} test set	12664 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.065 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3490	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: 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	0.47	0/1169	0.74	2/1583 (0.1%)
1	B	0.68	2/1163 (0.2%)	0.90	6/1575 (0.4%)
1	C	0.62	0/1169	0.97	6/1583 (0.4%)
All	All	0.60	2/3501 (0.1%)	0.88	14/4741 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	LYS	CD-CE	8.19	1.71	1.51
1	B	67	GLY	CA-C	5.52	1.60	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	22	LYS	CD-CE-NZ	10.73	136.37	111.70
1	C	70	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	C	22	LYS	CG-CD-CE	9.37	140.02	111.90
1	C	22	LYS	CA-CB-CG	8.46	132.01	113.40
1	B	121	GLN	CA-CB-CG	-7.71	96.43	113.40
1	B	135	ASP	C-N-CA	7.53	140.52	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	GLU	CG-CD-OE2	-6.93	104.44	118.30
1	B	121	GLN	CB-CG-CD	6.82	129.32	111.60
1	C	114	ASN	CB-CA-C	6.08	122.55	110.40
1	A	110	GLN	CB-CA-C	-5.70	99.00	110.40
1	A	110	GLN	CA-CB-CG	5.32	125.09	113.40
1	B	136	GLU	CG-CD-OE1	5.17	128.64	118.30
1	B	120	PRO	C-N-CA	-5.08	109.01	121.70
1	C	29	ARG	CB-CG-CD	5.06	124.76	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	ASP	Peptide
1	B	136	GLU	Sidechain
1	B	144	VAL	Peptide
1	C	29	ARG	Sidechain
1	C	35	GLN	Peptide

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	1141	0	1086	39	0
1	B	1136	0	1081	70	1
1	C	1141	0	1086	56	0
2	A	5	0	0	3	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
3	A	19	0	0	4	0
3	B	21	0	0	7	1
3	C	17	0	0	8	1
All	All	3490	0	3253	156	2

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 23.

All (156) 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:1:PRO:CB	2:B:201:SO4:O4	1.90	1.19
1:C:28:HIS:NE2	2:C:201:SO4:O4	1.82	1.13
1:B:1:PRO:HB3	2:B:201:SO4:O4	0.97	1.13
1:B:58:GLN:NE2	3:B:301:HOH:O	1.97	0.96
1:B:117:ARG:HH21	1:B:132:LEU:HG	1.36	0.90
1:C:125:GLU:O	3:C:301:HOH:O	1.93	0.86
1:C:63:ILE:HD11	1:C:95:ILE:HD12	1.58	0.86
1:A:137:ARG:O	1:A:141:GLU:HG3	1.79	0.81
1:B:9:GLN:HG2	1:B:47:PRO:HA	1.63	0.80
1:B:127:GLU:OE1	3:B:302:HOH:O	2.02	0.77
1:B:98:LYS:O	3:B:303:HOH:O	2.03	0.75
1:B:117:ARG:HE	1:B:132:LEU:CD1	2.01	0.74
1:B:126:GLY:O	3:B:304:HOH:O	2.06	0.73
1:A:124:HIS:HD1	1:A:127:GLU:HG3	1.54	0.73
1:B:40:GLN:HE21	1:B:42:ASN:HD22	1.36	0.73
1:B:25:THR:HG23	1:B:39:ALA:HB3	1.68	0.73
1:B:109:ALA:HB3	1:B:121:GLN:HE21	1.54	0.72
1:A:120:PRO:HB2	1:A:124:HIS:HB3	1.71	0.72
1:C:53:LEU:HD23	1:C:58:GLN:HG3	1.69	0.72
1:B:38:LEU:HD23	1:B:114:ASN:HD22	1.53	0.72
1:B:120:PRO:HG3	1:B:128:TRP:CG	2.25	0.72
1:C:128:TRP:HB3	3:C:301:HOH:O	1.89	0.71
1:B:11:ARG:HA	3:B:305:HOH:O	1.91	0.71
1:B:101:TRP:CD2	1:C:114:ASN:HB2	2.25	0.71
1:A:123:GLY:O	3:A:301:HOH:O	2.09	0.71
1:B:117:ARG:NH2	1:B:132:LEU:HG	2.06	0.70
1:B:29:ARG:HD2	1:B:36:HIS:CD2	2.27	0.70
1:C:53:LEU:HD23	1:C:58:GLN:CG	2.22	0.69
1:A:70:ARG:HD3	1:A:119:LEU:HD23	1.73	0.69
1:C:46:GLN:HB3	1:C:50:ASN:HD22	1.57	0.67
1:B:132:LEU:HD13	1:B:136:GLU:OE2	1.93	0.67
1:C:46:GLN:NE2	3:C:303:HOH:O	2.28	0.66
1:B:10:ASP:O	3:B:305:HOH:O	2.14	0.66
1:A:124:HIS:ND1	1:A:127:GLU:HG3	2.09	0.66
1:A:36:HIS:HB2	1:A:144:VAL:HG22	1.78	0.65
1:B:109:ALA:HB3	1:B:121:GLN:NE2	2.12	0.65
1:C:96:ASP:OD2	1:C:98:LYS:HG2	1.98	0.64
1:C:139:PHE:O	1:C:142:THR:OG1	2.14	0.64
1:C:36:HIS:HB3	1:C:144:VAL:HG22	1.80	0.63
1:B:121:GLN:O	1:B:124:HIS:N	2.31	0.62
1:C:28:HIS:CE1	2:C:201:SO4:O4	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:HIS:HB3	1:B:144:VAL:HG22	1.83	0.61
1:B:1:PRO:HD2	1:B:39:ALA:HA	1.83	0.61
1:B:40:GLN:NE2	1:B:42:ASN:HD22	1.99	0.60
1:B:117:ARG:HE	1:B:132:LEU:HG	1.67	0.59
1:A:2:VAL:HG13	1:A:40:GLN:HG2	1.83	0.59
1:A:114:ASN:CG	1:A:119:LEU:HD11	2.22	0.59
1:C:113:VAL:O	1:C:114:ASN:HB3	2.03	0.59
1:B:120:PRO:HG3	1:B:128:TRP:CB	2.33	0.58
1:B:120:PRO:HG3	1:B:128:TRP:HB2	1.85	0.58
1:B:31:LEU:HD12	1:B:81:LEU:HA	1.86	0.58
1:B:109:ALA:HA	1:B:112:MET:HG3	1.85	0.58
1:B:96:ASP:OD1	1:B:97:ARG:N	2.37	0.57
1:B:84:ARG:NH1	3:B:307:HOH:O	2.31	0.57
1:A:29:ARG:HE	1:A:36:HIS:CE1	2.23	0.56
1:B:130:ASP:N	1:B:131:ASN:OD1	2.38	0.56
1:C:40:GLN:HE21	1:C:42:ASN:HD22	1.52	0.56
1:C:128:TRP:HE3	3:C:301:HOH:O	1.88	0.56
1:C:8:SER:HA	1:C:46:GLN:O	2.05	0.56
1:C:116:GLY:O	1:C:117:ARG:HD2	2.05	0.56
1:B:64:PHE:CE2	1:C:2:VAL:HG11	2.40	0.56
1:B:132:LEU:HB2	1:B:136:GLU:HG3	1.88	0.56
1:C:46:GLN:HA	3:C:303:HOH:O	2.05	0.55
1:B:27:ALA:HB1	1:B:84:ARG:HD2	1.88	0.54
1:C:46:GLN:CD	3:C:303:HOH:O	2.45	0.54
1:B:129:PHE:HE1	1:B:140:MET:SD	2.31	0.54
1:C:40:GLN:NE2	1:C:42:ASN:HD22	2.06	0.54
1:C:4:MET:SD	1:C:42:ASN:HB3	2.49	0.53
1:C:29:ARG:HG2	1:C:30:GLY:N	2.21	0.53
1:C:63:ILE:HD12	1:C:100:ILE:HD12	1.90	0.53
1:B:117:ARG:HE	1:B:132:LEU:CG	2.21	0.53
1:C:25:THR:HG23	1:C:39:ALA:HB3	1.91	0.53
1:A:1:PRO:HB3	2:A:201:SO4:O4	2.09	0.52
1:B:108:PRO:O	1:B:111:GLN:HG2	2.06	0.52
1:C:133:SER:HB3	1:C:136:GLU:OE1	2.09	0.52
1:B:7:VAL:HG11	1:B:12:LEU:HD11	1.91	0.52
1:B:37:PHE:HB3	1:B:144:VAL:HG23	1.91	0.52
1:A:127:GLU:OE2	3:A:302:HOH:O	2.18	0.52
1:C:70:ARG:HD3	1:C:119:LEU:HD23	1.92	0.52
1:A:73:ARG:NH2	2:A:201:SO4:S	2.84	0.51
1:C:116:GLY:C	1:C:117:ARG:HD2	2.31	0.51
1:C:46:GLN:HB3	1:C:50:ASN:ND2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HB2	1:B:136:GLU:CG	2.40	0.51
1:A:7:VAL:HG12	1:A:63:ILE:HD13	1.91	0.51
1:C:113:VAL:O	1:C:114:ASN:CB	2.58	0.50
1:A:117:ARG:HH11	1:A:117:ARG:HB3	1.76	0.50
1:B:128:TRP:O	1:B:130:ASP:N	2.44	0.50
1:A:120:PRO:HG3	1:A:128:TRP:CG	2.47	0.50
1:A:32:THR:OG1	1:A:34:THR:HG23	2.11	0.50
1:B:130:ASP:O	1:B:133:SER:CB	2.60	0.49
1:B:132:LEU:HB2	1:B:136:GLU:OE2	2.12	0.49
1:B:108:PRO:O	1:B:112:MET:HG3	2.12	0.49
1:A:1:PRO:HG3	1:A:28:HIS:CD2	2.47	0.49
1:A:36:HIS:ND1	1:A:144:VAL:HG13	2.28	0.49
1:B:7:VAL:O	1:B:45:GLU:HA	2.12	0.49
1:C:122:PRO:HA	1:C:125:GLU:OE2	2.12	0.49
1:B:103:TYR:CE1	1:C:112:MET:HB3	2.48	0.48
1:A:143:ASN:O	1:C:54:GLY:HA3	2.13	0.48
1:B:29:ARG:HG3	1:B:30:GLY:N	2.28	0.48
1:A:7:VAL:HG12	1:A:63:ILE:CD1	2.43	0.48
1:B:104:PHE:O	1:C:107:MET:HG2	2.13	0.48
1:C:73:ARG:HB3	1:C:77:LEU:HD23	1.96	0.48
1:A:8:SER:HB2	1:A:60:GLY:O	2.14	0.48
1:C:4:MET:HB3	1:C:6:TYR:CE1	2.49	0.48
1:B:7:VAL:HG12	1:B:63:ILE:HG12	1.96	0.47
1:B:132:LEU:CD1	1:B:136:GLU:OE2	2.63	0.47
1:B:138:ALA:HA	1:B:141:GLU:HG2	1.97	0.47
1:C:96:ASP:OD2	1:C:98:LYS:HE3	2.14	0.47
1:B:31:LEU:HD21	1:B:84:ARG:HH21	1.80	0.47
1:A:123:GLY:O	1:A:124:HIS:HB2	2.15	0.47
1:B:36:HIS:CB	1:B:144:VAL:HG22	2.44	0.47
1:B:124:HIS:O	1:B:125:GLU:HB3	2.15	0.47
1:C:99:HIS:C	1:C:100:ILE:HD13	2.35	0.47
1:B:130:ASP:O	1:B:133:SER:HB3	2.14	0.47
1:B:1:PRO:HG3	1:B:28:HIS:CE1	2.50	0.46
1:A:131:ASN:OD1	1:A:131:ASN:N	2.48	0.46
1:B:133:SER:O	1:B:134:SER:HB3	2.16	0.46
1:C:17:LYS:HZ1	1:C:45:GLU:CD	2.19	0.46
1:B:109:ALA:H	1:B:121:GLN:NE2	2.14	0.46
1:B:56:VAL:HG23	1:C:145:ASP:HB2	1.97	0.46
1:A:11:ARG:HH12	1:A:95:ILE:CG1	2.29	0.46
1:A:101:TRP:CD1	1:A:101:TRP:N	2.84	0.45
1:C:1:PRO:N	3:C:302:HOH:O	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HA	3:A:306:HOH:O	2.16	0.45
1:B:117:ARG:NE	1:B:132:LEU:HG	2.31	0.44
1:A:120:PRO:HB2	1:A:124:HIS:CB	2.45	0.44
1:C:71:GLU:HG2	1:C:106:GLU:HB3	1.99	0.44
1:B:121:GLN:O	1:B:123:GLY:N	2.51	0.44
1:C:63:ILE:HD12	1:C:100:ILE:CD1	2.48	0.44
1:C:51:VAL:HG11	1:C:62:THR:HG21	1.98	0.43
1:A:2:VAL:HG23	1:C:103:TYR:CZ	2.54	0.43
1:C:37:PHE:HB3	1:C:144:VAL:HG23	2.01	0.42
1:B:52:PHE:CE2	1:B:57:GLN:HG3	2.54	0.42
1:C:100:ILE:HD13	1:C:100:ILE:N	2.34	0.42
1:B:25:THR:HG23	1:B:39:ALA:CB	2.43	0.42
1:B:27:ALA:CB	1:B:84:ARG:HD2	2.49	0.42
1:A:1:PRO:HD2	1:A:38:LEU:O	2.20	0.42
1:A:94:GLU:HG3	1:A:94:GLU:O	2.19	0.42
1:B:125:GLU:HA	1:B:128:TRP:HB3	2.01	0.41
1:A:70:ARG:O	3:A:303:HOH:O	2.21	0.41
1:A:73:ARG:NH2	2:A:201:SO4:O3	2.53	0.41
1:C:29:ARG:NH1	1:C:36:HIS:CD2	2.88	0.41
1:C:1:PRO:HG2	1:C:39:ALA:HA	2.01	0.41
1:B:6:TYR:CE1	1:C:4:MET:HE3	2.56	0.41
1:A:114:ASN:OD1	1:A:119:LEU:HD11	2.20	0.41
1:C:35:GLN:NE2	1:C:129:PHE:HB2	2.36	0.41
1:A:51:VAL:HG22	1:B:42:ASN:ND2	2.36	0.41
1:A:6:TYR:CD1	1:A:44:GLN:HB2	2.56	0.40
1:A:32:THR:HB	1:A:73:ARG:NH1	2.36	0.40
1:A:78:LYS:HZ3	1:A:106:GLU:CD	2.24	0.40
1:C:70:ARG:HA	1:C:107:MET:O	2.21	0.40
1:C:11:ARG:NH2	3:C:307:HOH:O	2.54	0.40
1:B:52:PHE:CD1	1:B:52:PHE:N	2.90	0.40
1:A:11:ARG:HH12	1:A:95:ILE:HG12	1.87	0.40
1:C:71:GLU:HG3	1:C:107:MET:C	2.42	0.40
1:C:87:ASP:O	1:C:90:SER:HB3	2.22	0.40

All (2) 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:B:13:THR:OG1	1:B:94:GLU:OE1[4_565]	1.92	0.28
3:B:318:HOH:O	3:C:316: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	143/165 (87%)	137 (96%)	5 (4%)	1 (1%)	19 35
1	B	143/165 (87%)	133 (93%)	5 (4%)	5 (4%)	3 4
1	C	143/165 (87%)	138 (96%)	3 (2%)	2 (1%)	9 17
All	All	429/495 (87%)	408 (95%)	13 (3%)	8 (2%)	6 12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	B	131	ASN
1	B	133	SER
1	B	134	SER
1	C	36	HIS
1	B	125	GLU
1	B	129	PHE
1	C	124	HIS

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	118/137 (86%)	111 (94%)	7 (6%)	16 33
1	B	117/137 (85%)	110 (94%)	7 (6%)	16 33
1	C	118/137 (86%)	108 (92%)	10 (8%)	8 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	353/411 (86%)	329 (93%)	24 (7%)	13 27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	22	LYS
1	A	98	LYS
1	A	110	GLN
1	A	130	ASP
1	A	131	ASN
1	A	135	ASP
1	B	1	PRO
1	B	26	ASP
1	B	29	ARG
1	B	90	SER
1	B	98	LYS
1	B	133	SER
1	B	137	ARG
1	C	4	MET
1	C	9	GLN
1	C	22	LYS
1	C	29	ARG
1	C	70	ARG
1	C	76	ASP
1	C	110	GLN
1	C	119	LEU
1	C	134	SER
1	C	145	ASP

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

Mol	Chain	Res	Type
1	A	42	ASN
1	A	50	ASN
1	B	36	HIS
1	B	40	GLN
1	B	44	GLN
1	B	114	ASN
1	B	121	GLN
1	C	40	GLN

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Mol	Chain	Res	Type
1	C	50	ASN
1	C	114	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 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	$\#\|Z\| > 2$
2	SO4	A	201	-	4,4,4	1.08	0	6,6,6	1.60	2 (33%)
2	SO4	C	201	-	4,4,4	1.20	0	6,6,6	0.68	0
2	SO4	B	201	-	4,4,4	1.09	0	6,6,6	0.73	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	SO4	O3-S-O1	-2.89	94.47	109.56
2	A	201	SO4	O3-S-O2	2.10	120.51	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	SO4	3	0
2	C	201	SO4	2	0
2	B	201	SO4	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

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	145/165 (87%)	0.12	4 (2%)	55	51	23, 37, 57, 68	0
1	B	145/165 (87%)	0.21	8 (5%)	32	29	22, 34, 61, 69	0
1	C	145/165 (87%)	0.04	2 (1%)	73	70	24, 37, 49, 71	0
All	All	435/495 (87%)	0.12	14 (3%)	50	47	22, 36, 57, 71	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	ASN	4.7
1	B	132	LEU	3.4
1	C	123	GLY	3.2
1	B	121	GLN	3.0
1	B	122	PRO	2.6
1	B	134	SER	2.5
1	A	126	GLY	2.5
1	A	124	HIS	2.5
1	B	123	GLY	2.5
1	C	142	THR	2.5
1	B	130	ASP	2.4
1	B	135	ASP	2.4
1	A	123	GLY	2.2
1	A	60	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	SO4	A	201	5/5	0.96	0.06	34,39,44,49	0
2	SO4	B	201	5/5	0.96	0.08	35,38,41,45	0
2	SO4	C	201	5/5	0.97	0.06	35,36,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.