



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 04:42 PM EDT

PDB ID : 1L9W  
Title : CRYSTAL STRUCTURE OF 3-DEHYDROQUINASE FROM SALMONELLA TYPHI COMPLEXED WITH REACTION PRODUCT  
Authors : Lee, W.H.; Perles, L.A.; Nagem, R.A.P.; Shrive, A.K.; Hawkins, A.; Sawyer, L.; Polikarpov, I.  
Deposited on : 2002-03-26  
Resolution : 2.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.35  
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) : 2.35

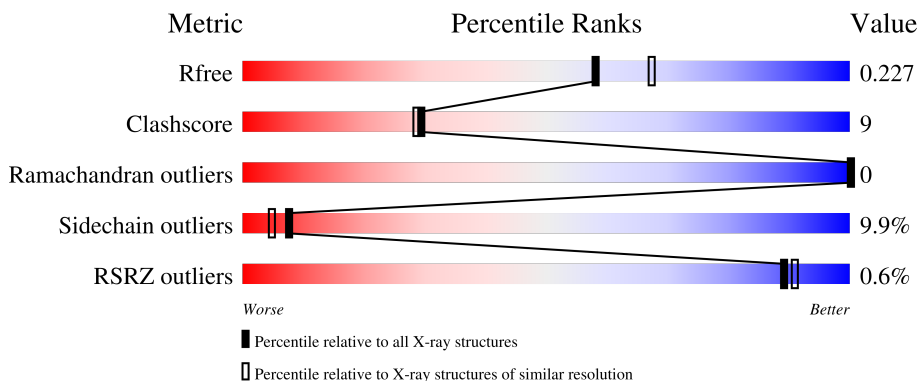
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	252	
1	B	252	
1	C	252	
1	D	252	

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	DHS	A	301	X	X	-	-
2	DHS	B	302	X	X	-	-
2	DHS	C	303	X	X	-	-
2	DHS	D	304	X	-	-	-

## 2 Entry composition [i](#)

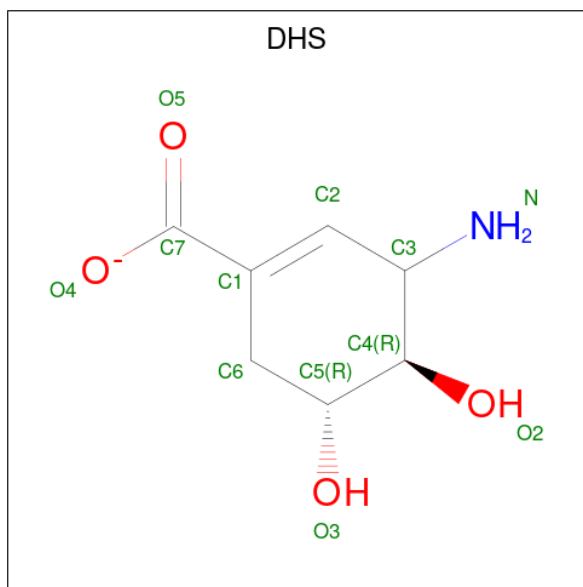
There are 3 unique types of molecules in this entry. The entry contains 7987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-dehydroquinate dehydratase aroD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	Total 1934	C 1219	N 335	O 366	S 14	0	0	0
1	B	252	Total 1934	C 1219	N 335	O 366	S 14	0	0	0
1	C	252	Total 1934	C 1219	N 335	O 366	S 14	0	0	0
1	D	252	Total 1934	C 1219	N 335	O 366	S 14	0	0	0

- Molecule 2 is 3-AMINO-4,5-DIHYDROXY-CYCLOHEX-1-ENECARBOXYLATE (three-letter code: DHS) (formula: C<sub>7</sub>H<sub>10</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 11	C 7	O 4	0	0
2	B	1	Total 11	C 7	O 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			11	7	4		
2	D	1	Total	C	O	0	0
			11	7	4		

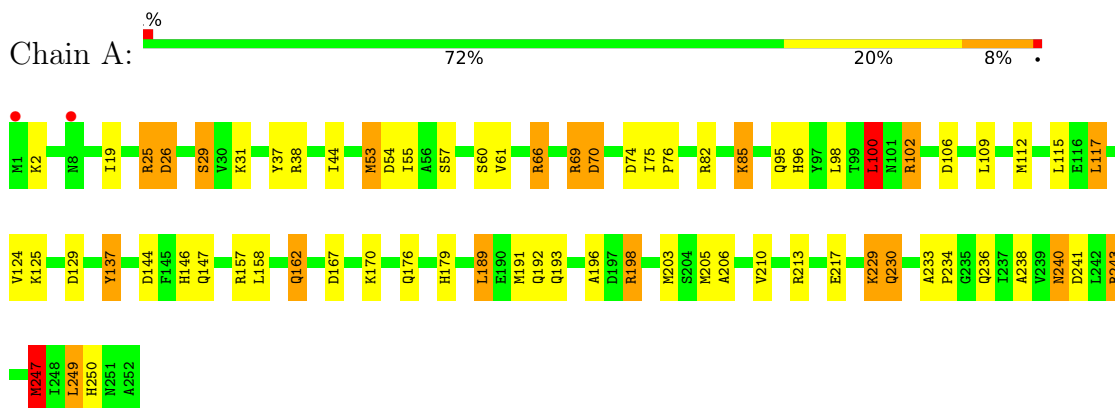
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	54	Total	O	1	0
			54	54		
3	C	44	Total	O	2	0
			44	44		
3	D	60	Total	O	5	0
			60	60		

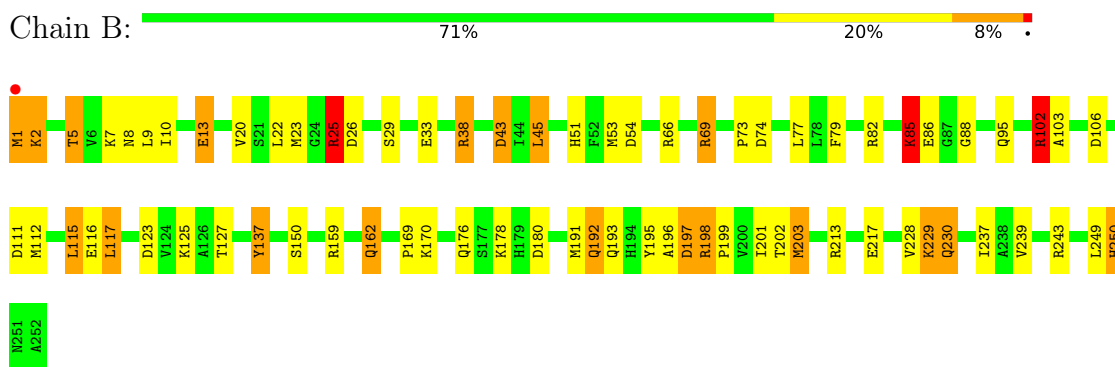
### 3 Residue-property plots [i](#)

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.

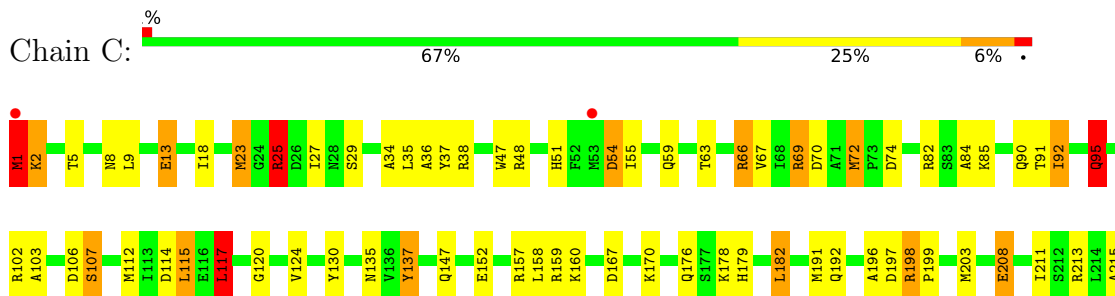
- Molecule 1: 3-dehydroquinate dehydratase aroD

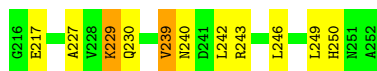


- Molecule 1: 3-dehydroquinate dehydratase aroD



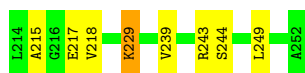
- Molecule 1: 3-dehydroquinate dehydratase aroD





- Molecule 1: 3-dehydroquinate dehydratase aroD

Chain D: 68% 24% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.61Å 158.56Å 85.89Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 75.9 (10.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.09Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.177 , 0.245 0.165 , 0.227	Depositor DCC
$R_{free}$ test set	2479 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 77.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DHS

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	0.89	0/1965	1.98	49/2661 (1.8%)
1	B	0.96	0/1965	2.05	55/2661 (2.1%)
1	C	0.88	0/1965	1.85	43/2661 (1.6%)
1	D	0.88	1/1965 (0.1%)	2.07	49/2661 (1.8%)
All	All	0.90	1/7860 (0.0%)	1.99	196/10644 (1.8%)

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	1
1	C	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	156	SER	CB-OG	5.19	1.49	1.42

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	ARG	NE-CZ-NH2	28.00	134.30	120.30
1	D	69	ARG	CD-NE-CZ	25.34	159.07	123.60
1	D	38	ARG	NE-CZ-NH1	-24.85	107.87	120.30
1	B	25	ARG	CD-NE-CZ	22.70	155.38	123.60
1	B	38	ARG	NE-CZ-NH1	-18.68	110.96	120.30
1	A	198	ARG	NE-CZ-NH2	-17.76	111.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASP	CB-CG-OD2	-17.69	102.38	118.30
1	A	198	ARG	NE-CZ-NH1	17.42	129.01	120.30
1	B	69	ARG	CD-NE-CZ	17.00	147.40	123.60
1	B	198	ARG	NE-CZ-NH2	-16.76	111.92	120.30
1	D	69	ARG	NE-CZ-NH1	16.59	128.59	120.30
1	A	25	ARG	CD-NE-CZ	16.46	146.64	123.60
1	B	69	ARG	NE-CZ-NH1	16.43	128.52	120.30
1	A	102	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	B	26	ASP	CB-CG-OD2	15.96	132.66	118.30
1	D	38	ARG	CD-NE-CZ	15.21	144.90	123.60
1	D	66	ARG	NE-CZ-NH1	15.13	127.86	120.30
1	C	157	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	D	198	ARG	NE-CZ-NH1	13.89	127.24	120.30
1	A	69	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	A	243	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	B	25	ARG	NE-CZ-NH1	12.27	126.44	120.30
1	B	38	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	C	213	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	A	157	ARG	NE-CZ-NH1	11.81	126.21	120.30
1	A	38	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	C	114	ASP	CB-CG-OD1	10.49	127.74	118.30
1	C	198	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	A	243	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	B	198	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	B	111	ASP	CB-CG-OD2	10.14	127.42	118.30
1	B	53	MET	CA-CB-CG	9.86	130.07	113.30
1	C	25	ARG	NE-CZ-NH2	9.83	125.21	120.30
1	B	137	TYR	CB-CG-CD1	9.80	126.88	121.00
1	A	157	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	B	213	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	54	ASP	CB-CG-OD1	9.54	126.88	118.30
1	A	25	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	B	69	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	D	48	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	123	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	B	54	ASP	CB-CG-OD1	9.13	126.52	118.30
1	B	180	ASP	CB-CG-OD1	-9.12	110.09	118.30
1	D	25	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	26	ASP	CB-CG-OD2	8.87	126.28	118.30
1	D	69	ARG	NH1-CZ-NH2	-8.56	109.98	119.40
1	C	69	ARG	CD-NE-CZ	8.41	135.37	123.60
1	D	106	ASP	CB-CG-OD1	8.40	125.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	CD-NE-CZ	8.38	135.33	123.60
1	A	70	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	A	106	ASP	CB-CG-OD2	8.27	125.74	118.30
1	A	26	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	B	102	ARG	CD-NE-CZ	8.12	134.97	123.60
1	C	117	LEU	CA-CB-CG	8.09	133.90	115.30
1	C	102	ARG	CD-NE-CZ	8.06	134.88	123.60
1	D	66	ARG	CD-NE-CZ	8.01	134.82	123.60
1	A	167	ASP	CB-CG-OD2	7.99	125.49	118.30
1	D	25	ARG	CD-NE-CZ	7.98	134.77	123.60
1	C	243	ARG	CD-NE-CZ	7.98	134.77	123.60
1	A	144	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	B	123	ASP	CB-CG-OD2	7.83	125.34	118.30
1	B	79	PHE	CB-CG-CD1	-7.77	115.36	120.80
1	A	25	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	159	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	C	157	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	144	ASP	CB-CG-OD1	7.60	125.14	118.30
1	C	167	ASP	CB-CG-OD2	7.57	125.11	118.30
1	D	198	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	66	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	D	82	ARG	CD-NE-CZ	7.48	134.07	123.60
1	B	111	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	B	243	ARG	NE-CZ-NH1	-7.45	116.57	120.30
1	C	13	GLU	CA-CB-CG	7.42	129.73	113.40
1	A	74	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	48	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	B	43	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	D	243	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	C	159	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	D	102	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	70	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	240	ASN	CA-CB-CG	-6.89	98.24	113.40
1	D	215	ALA	CB-CA-C	-6.81	99.88	110.10
1	B	197	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	189	LEU	CB-CG-CD2	6.76	122.49	111.00
1	C	38	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	C	159	ARG	CD-NE-CZ	6.68	132.95	123.60
1	C	74	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	C	54	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	13	GLU	OE1-CD-OE2	6.58	131.19	123.30
1	B	106	ASP	CB-CG-OD1	-6.54	112.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	213	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	140	MET	CG-SD-CE	6.50	110.61	100.20
1	C	213	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	85	LYS	CB-CG-CD	6.46	128.40	111.60
1	A	60	SER	N-CA-CB	6.42	120.14	110.50
1	B	198	ARG	CD-NE-CZ	6.41	132.58	123.60
1	A	117	LEU	CB-CG-CD2	6.40	121.88	111.00
1	A	146	HIS	CA-CB-CG	-6.39	102.74	113.60
1	A	249	LEU	CA-CB-CG	6.35	129.91	115.30
1	B	45	LEU	CD1-CG-CD2	-6.35	91.45	110.50
1	C	167	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	D	213	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	137	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	A	137	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	179	HIS	CA-CB-CG	-6.23	103.01	113.60
1	B	117	LEU	CB-CG-CD2	6.21	121.56	111.00
1	B	1	MET	CA-CB-CG	6.14	123.75	113.30
1	B	74	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	116	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	B	230	GLN	CB-CG-CD	6.06	127.36	111.60
1	B	13	GLU	CA-CB-CG	6.04	126.70	113.40
1	B	26	ASP	OD1-CG-OD2	-5.98	111.94	123.30
1	A	210	VAL	O-C-N	-5.96	113.16	122.70
1	D	82	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	197	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	D	66	ARG	NH1-CZ-NH2	-5.95	112.86	119.40
1	B	150	SER	N-CA-CB	-5.93	101.60	110.50
1	C	48	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	C	95	GLN	CB-CG-CD	5.91	126.97	111.60
1	A	69	ARG	CD-NE-CZ	5.90	131.87	123.60
1	B	103	ALA	N-CA-CB	5.90	118.36	110.10
1	C	137	TYR	CA-CB-CG	-5.89	102.20	113.40
1	D	82	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	215	ALA	CB-CA-C	-5.83	101.36	110.10
1	A	82	ARG	CD-NE-CZ	5.80	131.72	123.60
1	D	15	MET	N-CA-CB	-5.79	100.17	110.60
1	B	180	ASP	OD1-CG-OD2	5.79	134.29	123.30
1	C	107	SER	O-C-N	-5.79	113.36	123.20
1	B	8	ASN	CA-CB-CG	-5.76	100.72	113.40
1	D	74	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	250	HIS	O-C-N	-5.75	113.49	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	95	GLN	CB-CG-CD	5.72	126.48	111.60
1	D	43	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	B	191	MET	CA-C-O	5.68	132.02	120.10
1	D	157	ARG	CD-NE-CZ	5.65	131.51	123.60
1	C	179	HIS	CA-CB-CG	-5.62	104.04	113.60
1	D	26	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	D	198	ARG	CD-NE-CZ	5.61	131.46	123.60
1	B	95	GLN	OE1-CD-NE2	-5.59	109.05	121.90
1	B	79	PHE	O-C-N	-5.55	113.81	122.70
1	B	213	ARG	CG-CD-NE	5.53	123.40	111.80
1	B	38	ARG	CD-NE-CZ	-5.48	115.93	123.60
1	D	180	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	D	26	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	106	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	159	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	100	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	D	111	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	53	MET	CA-CB-CG	5.37	122.44	113.30
1	D	91	THR	N-CA-CB	5.37	120.50	110.30
1	A	66	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	57	SER	N-CA-CB	-5.35	102.47	110.50
1	C	2	LYS	CA-CB-CG	5.35	125.16	113.40
1	D	183	THR	OG1-CB-CG2	-5.34	97.71	110.00
1	D	50	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	102	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	79	PHE	CB-CG-CD2	5.30	124.51	120.80
1	A	129	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	116	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	A	69	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	16	PRO	N-CA-CB	5.27	109.63	103.30
1	A	74	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	82	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	C	1	MET	CA-C-O	5.22	131.07	120.10
1	C	197	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	137	TYR	CG-CD2-CE2	-5.22	117.13	121.30
1	C	92	ILE	CA-CB-CG1	5.20	120.88	111.00
1	A	213	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	66	ARG	CB-CA-C	-5.19	100.03	110.40
1	A	213	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	195	TYR	CB-CG-CD2	-5.17	117.89	121.00
1	C	103	ALA	N-CA-CB	-5.16	102.87	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	VAL	N-CA-CB	5.16	122.85	111.50
1	B	243	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	D	151	ALA	N-CA-CB	5.13	117.28	110.10
1	A	162	GLN	CA-CB-CG	5.13	124.68	113.40
1	B	203	MET	N-CA-CB	5.12	119.83	110.60
1	A	137	TYR	CA-CB-CG	-5.12	103.67	113.40
1	C	36	ALA	CB-CA-C	-5.11	102.43	110.10
1	D	57	SER	N-CA-CB	-5.11	102.83	110.50
1	B	5	THR	O-C-N	5.11	130.87	122.70
1	A	247	MET	CA-CB-CG	5.10	121.98	113.30
1	C	37	TYR	CB-CG-CD1	5.10	124.06	121.00
1	D	129	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	247	MET	O-C-N	5.10	130.86	122.70
1	D	79	PHE	N-CA-CB	-5.09	101.43	110.60
1	C	137	TYR	CZ-CE2-CD2	-5.09	115.22	119.80
1	C	59	GLN	CB-CG-CD	5.08	124.82	111.60
1	D	95	GLN	OE1-CD-NE2	-5.07	110.25	121.90
1	C	130	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	C	23	MET	CA-C-N	5.04	126.28	116.20
1	D	135	ASN	CB-CG-ND2	5.03	128.78	116.70
1	C	47	TRP	O-C-N	-5.03	114.65	122.70
1	A	124	VAL	N-CA-CB	5.02	122.55	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	ASP	Mainchain
1	C	107	SER	Mainchain
1	C	115	LEU	Mainchain
1	C	84	ALA	Mainchain

## 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	1934	0	1963	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1934	0	1963	40	0
1	C	1934	0	1963	42	0
1	D	1934	0	1963	35	0
2	A	11	0	7	3	0
2	B	11	0	7	1	0
2	C	11	0	6	1	0
2	D	11	0	6	0	0
3	A	49	0	0	1	0
3	B	54	0	0	2	1
3	C	44	0	0	2	1
3	D	60	0	0	9	0
All	All	7987	0	7878	147	1

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 (147) 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:25:ARG:HH21	1:B:51:HIS:HB3	1.23	1.04
1:D:95:GLN:NE2	3:D:305:HOH:O	1.98	0.91
1:C:211:ILE:HD11	1:D:211:ILE:HD11	1.55	0.88
1:B:25:ARG:NH2	1:B:51:HIS:HB3	1.96	0.79
1:D:85:LYS:HE2	1:D:86:GLU:HG3	1.64	0.78
1:C:227:ALA:O	1:C:239:VAL:HG22	1.85	0.77
1:D:112:MET:HG2	1:D:137:TYR:HB2	1.67	0.76
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.54	0.71
1:A:240:ASN:N	1:A:240:ASN:HD22	1.89	0.70
1:C:176:GLN:OE1	3:C:341:HOH:O	2.09	0.70
1:B:162:GLN:HE22	1:B:196:ALA:HA	1.56	0.70
1:A:217:GLU:OE2	1:A:250:HIS:HD2	1.76	0.68
1:C:208:GLU:HG3	3:C:345:HOH:O	1.91	0.68
1:D:25:ARG:HG3	1:D:53:MET:HG3	1.75	0.68
1:B:230:GLN:HG2	3:B:346:HOH:O	1.94	0.67
1:D:66:ARG:NE	3:D:324:HOH:O	2.21	0.67
1:D:86:GLU:OE2	3:D:311:HOH:O	2.12	0.67
1:D:85:LYS:HE2	1:D:86:GLU:CG	2.28	0.64
1:D:120:GLY:O	1:D:124:VAL:HG13	1.98	0.64
1:C:95:GLN:H	1:C:95:GLN:CD	2.02	0.63
1:B:217:GLU:OE2	1:B:250:HIS:HD2	1.82	0.62
1:A:243:ARG:O	1:A:247:MET:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASP:OD2	1:D:160:LYS:NZ	2.32	0.62
1:B:85:LYS:HE2	1:B:86:GLU:HG3	1.83	0.61
1:D:149:PRO:HD2	1:D:173:VAL:HG11	1.83	0.61
1:C:63:THR:O	1:C:67:VAL:HG23	2.00	0.60
1:C:217:GLU:OE2	1:C:250:HIS:HD2	1.85	0.59
1:C:66:ARG:NH1	1:C:70:ASP:OD1	2.32	0.59
1:A:96:HIS:HE1	3:A:329:HOH:O	1.85	0.59
1:C:55:ILE:HD12	1:C:92:ILE:HG21	1.85	0.58
1:A:217:GLU:OE2	1:A:250:HIS:CD2	2.56	0.58
1:D:55:ILE:HD11	1:D:90:GLN:NE2	2.19	0.58
1:C:120:GLY:O	1:C:124:VAL:HG22	2.03	0.57
1:C:25:ARG:NH2	1:C:51:HIS:ND1	2.52	0.57
1:A:240:ASN:HD22	1:A:240:ASN:H	1.52	0.56
1:C:229:LYS:HB3	1:C:229:LYS:NZ	2.19	0.56
1:B:162:GLN:HE21	1:B:198:ARG:HG2	1.70	0.56
1:D:198:ARG:HB2	1:D:199:PRO:HD2	1.87	0.56
1:C:229:LYS:HG3	1:C:230:GLN:H	1.70	0.56
1:D:66:ARG:NH2	3:D:326:HOH:O	2.23	0.55
1:C:229:LYS:HG3	1:C:230:GLN:HG2	1.87	0.55
1:B:228:VAL:HG12	1:B:229:LYS:HG3	1.89	0.55
1:A:112:MET:HG2	1:A:137:TYR:HB2	1.88	0.55
1:B:192:GLN:HG3	1:B:193:GLN:N	2.23	0.54
1:C:112:MET:HG2	1:C:137:TYR:HB2	1.89	0.54
1:D:229:LYS:HG3	3:D:356:HOH:O	2.06	0.54
1:D:170:LYS:HA	1:D:201:ILE:O	2.08	0.53
1:A:75:ILE:HD12	1:A:75:ILE:N	2.23	0.53
1:D:155:VAL:O	1:D:159:ARG:HG3	2.08	0.53
1:B:23:MET:CE	1:B:230:GLN:HG3	2.38	0.52
1:B:82:ARG:O	1:B:88:GLY:HA3	2.09	0.52
1:B:38:ARG:NH1	1:C:135:ASN:OD1	2.34	0.52
1:A:240:ASN:N	1:A:240:ASN:ND2	2.56	0.52
1:A:158:LEU:HD13	1:A:191:MET:HG2	1.92	0.52
1:A:240:ASN:H	1:A:240:ASN:ND2	2.07	0.52
1:D:38:ARG:HD3	3:D:321:HOH:O	2.10	0.52
1:B:5:THR:HG23	1:B:9:LEU:O	2.09	0.52
1:B:115:LEU:HD21	1:B:127:THR:HB	1.92	0.52
1:D:38:ARG:NE	3:D:342:HOH:O	2.13	0.51
1:B:85:LYS:HE2	1:B:86:GLU:CG	2.41	0.51
1:B:2:LYS:HB3	1:B:197:ASP:O	2.11	0.51
1:B:102:ARG:HG2	1:B:102:ARG:NH1	2.24	0.51
1:C:55:ILE:HG12	1:C:90:GLN:HE22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:MET:HE3	1:B:230:GLN:HG3	1.92	0.50
1:C:18:ILE:HD11	1:C:246:LEU:HD12	1.93	0.50
1:B:20:VAL:CG1	1:B:239:VAL:HG11	2.42	0.49
1:D:25:ARG:HH21	1:D:51:HIS:HB3	1.78	0.49
1:A:162:GLN:HE22	1:A:196:ALA:HA	1.78	0.48
1:C:34:ALA:HB1	1:C:72:MET:HE1	1.95	0.48
1:D:16:PRO:HD3	1:D:217:GLU:HB2	1.95	0.48
1:D:113:ILE:HD12	1:D:115:LEU:HD13	1.95	0.48
1:A:37:TYR:HE1	1:A:229:LYS:HE2	1.79	0.48
1:B:45:LEU:HD22	1:B:77:LEU:HD13	1.95	0.48
1:B:45:LEU:C	1:B:45:LEU:HD23	2.34	0.48
1:A:189:LEU:HD13	1:A:189:LEU:O	2.14	0.48
1:C:178:LYS:HD3	1:D:218:VAL:O	2.13	0.48
1:A:85:LYS:H	1:A:85:LYS:HD3	1.78	0.47
1:B:33:GLU:OE2	1:B:229:LYS:HE2	2.14	0.47
1:B:7:LYS:HE3	1:B:73:PRO:O	2.15	0.47
1:C:1:MET:HE3	1:C:196:ALA:HB1	1.97	0.47
1:C:55:ILE:HD11	1:C:90:GLN:NE2	2.30	0.47
1:C:242:LEU:O	1:C:246:LEU:HG	2.15	0.47
1:A:98:LEU:O	1:A:102:ARG:HG3	2.15	0.46
1:D:1:MET:HE3	1:D:196:ALA:HB1	1.98	0.46
1:A:66:ARG:NH1	1:A:70:ASP:OD1	2.42	0.45
1:A:162:GLN:HG3	1:A:198:ARG:NE	2.32	0.45
1:C:158:LEU:HD13	1:C:191:MET:HG2	1.98	0.45
1:D:200:VAL:HG12	1:D:201:ILE:N	2.31	0.45
1:A:162:GLN:HG3	1:A:198:ARG:CZ	2.47	0.45
1:B:170:LYS:HZ3	2:B:302:DHS:C3	2.30	0.45
1:B:198:ARG:HB2	1:B:199:PRO:CD	2.46	0.45
1:D:95:GLN:CG	3:D:305:HOH:O	2.65	0.45
1:C:66:ARG:HD2	1:C:70:ASP:OD1	2.17	0.45
1:B:162:GLN:NE2	1:B:197:ASP:H	2.15	0.44
1:A:205:MET:O	1:A:206:ALA:HB3	2.18	0.44
1:C:8:ASN:OD1	1:C:8:ASN:N	2.50	0.44
1:C:1:MET:HB3	1:C:2:LYS:H	1.36	0.44
1:A:19:ILE:HG12	1:A:44:ILE:HB	2.00	0.44
1:D:25:ARG:NH2	1:D:51:HIS:ND1	2.66	0.44
1:A:233:ALA:HB1	1:A:234:PRO:HD2	2.00	0.43
1:A:240:ASN:ND2	1:A:241:ASP:H	2.15	0.43
1:C:170:LYS:HZ3	2:C:303:DHS:C3	2.31	0.43
1:A:26:ASP:OD2	1:A:29:SER:OG	2.35	0.43
1:A:61:VAL:HG11	1:A:100:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HZ1	2:A:301:DHS:H2	1.83	0.43
1:C:27:ILE:H	1:C:27:ILE:HG13	1.58	0.43
1:A:170:LYS:HZ3	2:A:301:DHS:C3	2.31	0.43
1:B:162:GLN:HG2	1:B:198:ARG:CZ	2.48	0.43
1:C:55:ILE:CG1	1:C:90:GLN:HE22	2.31	0.43
1:C:117:LEU:HD21	1:C:160:LYS:HG2	1.99	0.43
1:D:140:MET:HE3	1:D:166:ALA:HB2	2.00	0.43
1:A:236:GLN:NE2	2:A:301:DHS:O5	2.47	0.43
1:B:2:LYS:HB3	1:B:2:LYS:HE3	1.85	0.43
1:B:162:GLN:HE22	1:B:197:ASP:H	1.65	0.43
1:C:198:ARG:HB2	1:C:199:PRO:HD2	2.00	0.43
1:B:202:THR:O	3:B:339:HOH:O	2.21	0.43
1:A:69:ARG:HD2	1:A:109:LEU:O	2.19	0.42
1:A:230:GLN:HE21	1:A:230:GLN:HB3	1.65	0.42
1:B:170:LYS:HA	1:B:201:ILE:O	2.18	0.42
1:C:23:MET:CE	1:C:230:GLN:HG3	2.49	0.42
1:D:2:LYS:HB3	1:D:2:LYS:HE3	1.94	0.42
1:A:55:ILE:H	1:A:55:ILE:HG13	1.46	0.42
1:D:140:MET:CE	1:D:166:ALA:HB2	2.50	0.42
1:D:184:LEU:C	1:D:184:LEU:HD13	2.40	0.42
1:C:92:ILE:HG21	1:C:92:ILE:HD13	1.90	0.42
1:B:112:MET:HG2	1:B:137:TYR:HB2	2.02	0.42
1:C:34:ALA:HB1	1:C:72:MET:CE	2.50	0.42
1:A:75:ILE:HG22	1:A:76:PRO:O	2.20	0.41
1:B:20:VAL:HG11	1:B:239:VAL:HG11	2.01	0.41
1:C:55:ILE:CD1	1:C:92:ILE:HG21	2.49	0.41
1:C:5:THR:HA	1:C:9:LEU:O	2.19	0.41
1:A:53:MET:HA	1:A:53:MET:CE	2.50	0.41
1:B:162:GLN:HG2	1:B:198:ARG:NE	2.36	0.41
1:B:198:ARG:HB2	1:B:199:PRO:HD2	2.02	0.41
1:A:189:LEU:HD11	1:A:193:GLN:OE1	2.20	0.41
1:A:238:ALA:HB1	1:A:240:ASN:HD21	1.84	0.41
1:B:38:ARG:NH1	1:C:135:ASN:HA	2.36	0.41
1:C:66:ARG:HD2	1:C:66:ARG:HH11	1.64	0.41
1:C:69:ARG:O	1:C:69:ARG:HG3	2.21	0.41
1:C:178:LYS:HZ2	1:C:178:LYS:HG2	1.51	0.41
1:B:22:LEU:C	1:B:22:LEU:HD23	2.40	0.41
1:B:169:PRO:HD2	1:B:199:PRO:O	2.22	0.40
1:B:102:ARG:HH11	1:B:102:ARG:CG	2.27	0.40
1:D:25:ARG:NH2	1:D:51:HIS:HB3	2.36	0.40
1:C:182:LEU:HD11	1:D:186:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLN:HG3	1:D:193:GLN:N	2.37	0.40
1:D:38:ARG:NH1	3:D:342:HOH:O	2.53	0.40

All (1) 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)
3:B:352:HOH:O	3:C:324:HOH:O[1_655]	2.18	0.02

## 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	250/252 (99%)	246 (98%)	4 (2%)	0	100	100
1	B	250/252 (99%)	242 (97%)	8 (3%)	0	100	100
1	C	250/252 (99%)	245 (98%)	5 (2%)	0	100	100
1	D	250/252 (99%)	243 (97%)	7 (3%)	0	100	100
All	All	1000/1008 (99%)	976 (98%)	24 (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	209/209 (100%)	191 (91%)	18 (9%)	10	7
1	B	209/209 (100%)	189 (90%)	20 (10%)	8	5
1	C	209/209 (100%)	188 (90%)	21 (10%)	7	5
1	D	209/209 (100%)	185 (88%)	24 (12%)	5	3
All	All	836/836 (100%)	753 (90%)	83 (10%)	8	5

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	25	ARG
1	A	29	SER
1	A	31	LYS
1	A	85	LYS
1	A	100	LEU
1	A	115	LEU
1	A	117	LEU
1	A	125	LYS
1	A	147	GLN
1	A	176	GLN
1	A	192	GLN
1	A	203	MET
1	A	229	LYS
1	A	230	GLN
1	A	240	ASN
1	A	247	MET
1	A	249	LEU
1	B	1	MET
1	B	2	LYS
1	B	10	ILE
1	B	13	GLU
1	B	25	ARG
1	B	29	SER
1	B	69	ARG
1	B	85	LYS
1	B	102	ARG
1	B	115	LEU
1	B	117	LEU
1	B	125	LYS
1	B	162	GLN
1	B	176	GLN
1	B	178	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	192	GLN
1	B	203	MET
1	B	229	LYS
1	B	237	ILE
1	B	249	LEU
1	C	1	MET
1	C	13	GLU
1	C	25	ARG
1	C	29	SER
1	C	35	LEU
1	C	54	ASP
1	C	72	MET
1	C	85	LYS
1	C	91	THR
1	C	95	GLN
1	C	115	LEU
1	C	117	LEU
1	C	147	GLN
1	C	152	GLU
1	C	182	LEU
1	C	192	GLN
1	C	203	MET
1	C	208	GLU
1	C	229	LYS
1	C	239	VAL
1	C	249	LEU
1	D	1	MET
1	D	2	LYS
1	D	13	GLU
1	D	25	ARG
1	D	29	SER
1	D	38	ARG
1	D	69	ARG
1	D	85	LYS
1	D	91	THR
1	D	115	LEU
1	D	117	LEU
1	D	125	LYS
1	D	147	GLN
1	D	156	SER
1	D	160	LYS
1	D	182	LEU

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Mol	Chain	Res	Type
1	D	192	GLN
1	D	203	MET
1	D	207	LYS
1	D	208	GLU
1	D	229	LYS
1	D	239	VAL
1	D	244	SER
1	D	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	162	GLN
1	A	230	GLN
1	A	240	ASN
1	A	250	HIS
1	B	162	GLN
1	B	250	HIS
1	C	90	GLN
1	C	162	GLN
1	C	250	HIS
1	D	90	GLN
1	D	162	GLN
1	D	250	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 monosaccharides in this entry.

## 5.6 Ligand geometry

4 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	DHS	D	304	1	11,11,12	2.82	4 (36%)	12,15,17	4.54	8 (66%)
2	DHS	C	303	1	11,11,12	2.64	5 (45%)	12,15,17	6.83	10 (83%)
2	DHS	B	302	1	11,11,12	2.45	3 (27%)	12,15,17	4.14	11 (91%)
2	DHS	A	301	1	11,11,12	2.92	5 (45%)	12,15,17	5.58	9 (75%)

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	DHS	D	304	1	1/1/4/6	4/4/17/20	0/1/1/1
2	DHS	C	303	1	2/2/4/6	4/4/17/20	0/1/1/1
2	DHS	B	302	1	2/2/4/6	4/4/17/20	0/1/1/1
2	DHS	A	301	1	2/2/4/6	4/4/17/20	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	DHS	C3-C4	6.90	1.60	1.52
2	B	302	DHS	C3-C4	6.54	1.60	1.52
2	A	301	DHS	C3-C4	6.39	1.59	1.52
2	C	303	DHS	C6-C1	4.85	1.59	1.51
2	C	303	DHS	C3-C2	4.80	1.60	1.50
2	D	304	DHS	C3-C2	3.83	1.58	1.50
2	A	301	DHS	C5-C4	3.61	1.57	1.52
2	A	301	DHS	C3-C2	3.51	1.57	1.50
2	B	302	DHS	C3-C2	3.11	1.56	1.50
2	A	301	DHS	C7-C1	3.05	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	DHS	C5-C4	3.03	1.56	1.52
2	A	301	DHS	C6-C1	2.86	1.56	1.51
2	C	303	DHS	C5-C4	2.83	1.56	1.52
2	D	304	DHS	C6-C5	-2.42	1.48	1.52
2	C	303	DHS	C3-C4	2.28	1.55	1.52
2	C	303	DHS	C6-C5	-2.19	1.49	1.52
2	B	302	DHS	C6-C5	2.05	1.56	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	DHS	O3-C5-C6	10.64	133.16	109.53
2	C	303	DHS	C3-C2-C1	-10.63	100.93	122.93
2	A	301	DHS	O2-C4-C5	-10.12	87.80	110.22
2	C	303	DHS	O2-C4-C5	-10.01	88.04	110.22
2	C	303	DHS	C6-C1-C2	-8.87	101.84	119.68
2	A	301	DHS	O3-C5-C6	8.63	128.71	109.53
2	B	302	DHS	C3-C2-C1	-8.24	105.88	122.93
2	D	304	DHS	C3-C2-C1	-8.18	105.99	122.93
2	A	301	DHS	C6-C1-C2	-8.09	103.40	119.68
2	A	301	DHS	C3-C2-C1	-7.59	107.22	122.93
2	D	304	DHS	O3-C5-C6	7.49	126.17	109.53
2	D	304	DHS	O2-C4-C5	-7.35	93.94	110.22
2	C	303	DHS	O2-C4-C3	6.96	121.38	109.52
2	B	302	DHS	O4-C7-O5	-6.42	108.92	123.61
2	C	303	DHS	O4-C7-C1	6.00	128.21	115.49
2	A	301	DHS	O4-C7-O5	-5.94	110.01	123.61
2	C	303	DHS	O5-C7-C1	-5.33	112.40	121.59
2	D	304	DHS	C5-C6-C1	5.07	121.68	111.78
2	C	303	DHS	C6-C1-C7	-4.08	109.26	116.91
2	C	303	DHS	O3-C5-C4	-4.02	101.30	110.22
2	B	302	DHS	O2-C4-C3	3.95	116.25	109.52
2	B	302	DHS	O3-C5-C4	3.82	118.68	110.22
2	B	302	DHS	O3-C5-C6	3.69	117.73	109.53
2	D	304	DHS	O4-C7-O5	-3.60	115.36	123.61
2	A	301	DHS	O5-C7-C1	-3.60	115.39	121.59
2	B	302	DHS	C6-C1-C2	-3.51	112.61	119.68
2	D	304	DHS	O2-C4-C3	3.50	115.48	109.52
2	D	304	DHS	O4-C7-C1	3.23	122.34	115.49
2	B	302	DHS	O4-C7-C1	3.17	122.20	115.49
2	B	302	DHS	C5-C6-C1	-3.12	105.68	111.78
2	A	301	DHS	C6-C1-C7	-2.88	111.51	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	DHS	O2-C4-C5	-2.74	104.14	110.22
2	A	301	DHS	O4-C7-C1	2.69	121.19	115.49
2	B	302	DHS	O5-C7-C1	-2.66	117.00	121.59
2	A	301	DHS	O2-C4-C3	2.65	114.03	109.52
2	B	302	DHS	C3-C4-C5	-2.30	107.77	110.69
2	C	303	DHS	O4-C7-O5	-2.25	118.45	123.61
2	D	304	DHS	C6-C1-C2	-2.23	115.19	119.68

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	DHS	C4
2	A	301	DHS	C5
2	B	302	DHS	C4
2	B	302	DHS	C5
2	C	303	DHS	C4
2	C	303	DHS	C5
2	D	304	DHS	C4

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	DHS	C6-C1-C7-O4
2	A	301	DHS	C6-C1-C7-O5
2	A	301	DHS	C2-C1-C7-O5
2	B	302	DHS	C6-C1-C7-O4
2	B	302	DHS	C6-C1-C7-O5
2	B	302	DHS	C2-C1-C7-O4
2	C	303	DHS	C6-C1-C7-O4
2	C	303	DHS	C6-C1-C7-O5
2	C	303	DHS	C2-C1-C7-O4
2	D	304	DHS	C6-C1-C7-O4
2	D	304	DHS	C6-C1-C7-O5
2	D	304	DHS	C2-C1-C7-O4
2	D	304	DHS	C2-C1-C7-O5
2	A	301	DHS	C2-C1-C7-O4
2	B	302	DHS	C2-C1-C7-O5
2	C	303	DHS	C2-C1-C7-O5

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303	DHS	1	0
2	B	302	DHS	1	0
2	A	301	DHS	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	252/252 (100%)	-0.60	2 (0%) 86 88	15, 27, 43, 76	0
1	B	252/252 (100%)	-0.60	1 (0%) 92 93	15, 27, 43, 77	0
1	C	252/252 (100%)	-0.50	2 (0%) 86 88	18, 29, 44, 66	0
1	D	252/252 (100%)	-0.57	1 (0%) 92 93	18, 29, 44, 73	0
All	All	1008/1008 (100%)	-0.56	6 (0%) 89 91	15, 28, 44, 77	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	8.8
1	B	1	MET	6.2
1	A	1	MET	3.9
1	C	53	MET	2.9
1	A	8	ASN	2.8
1	C	1	MET	2.2

### 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	DHS	D	304	11/12	0.83	0.14	21,32,37,38	0
2	DHS	C	303	11/12	0.88	0.12	27,31,33,33	0
2	DHS	A	301	11/12	0.92	0.10	24,28,29,30	0
2	DHS	B	302	11/12	0.93	0.10	21,29,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.