



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:16 pm BST

PDB ID : 6NL2  
Title : Apo NIS synthetase DesD variant R306Q  
Authors : Hoffmann, K.M.  
Deposited on : 2019-01-07  
Resolution : 1.92 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.

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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 : 2.11  
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) : 2.11

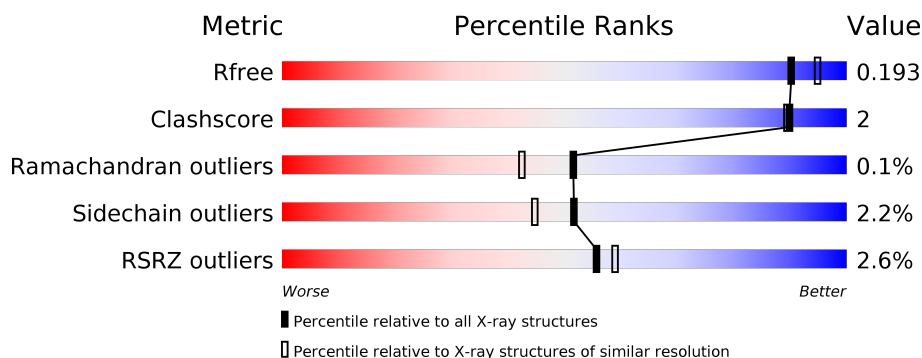
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on 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	594	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>•</div> </div> </div>
1	B	594	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10211 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 desferrioxamine E biosynthesis protein DesD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	3	0
			4704	2993	811	885	15			
1	B	593	Total	C	N	O	S	0	4	0
			4701	2991	811	884	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	GLN	ARG	engineered mutation	UNP Q9L069
A	596	GLY	-	expression tag	UNP Q9L069
B	306	GLN	ARG	engineered mutation	UNP Q9L069
B	596	GLY	-	expression tag	UNP Q9L069

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	371	Total	O	0	0
			371	371		

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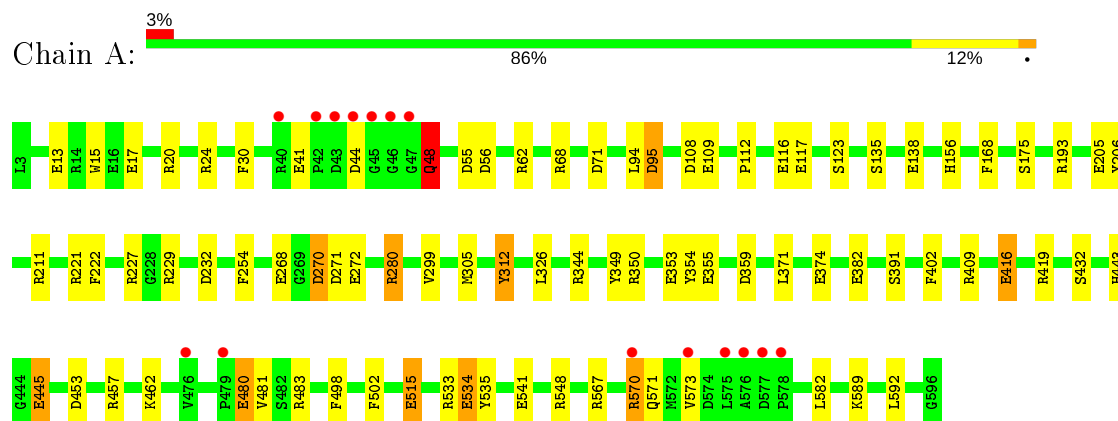
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	366	Total	O	0	0
			366	366		

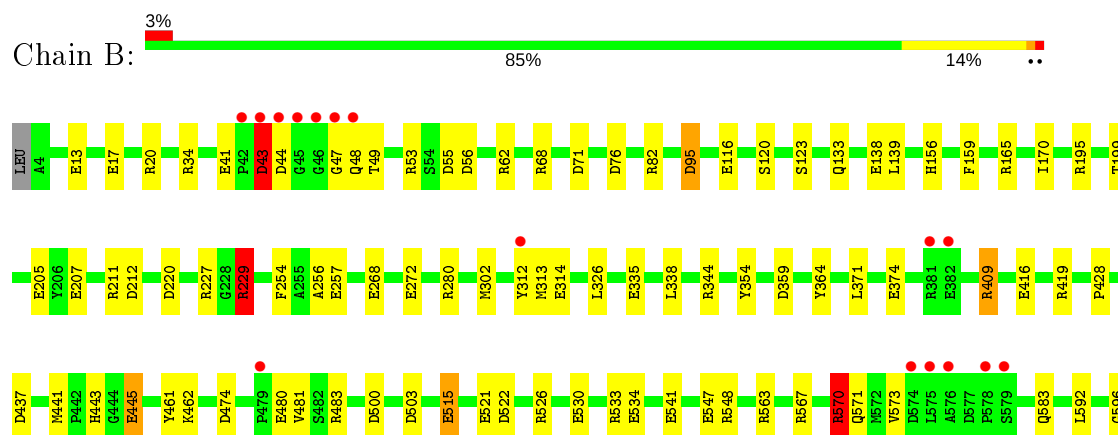
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: desferrioxamine E biosynthesis protein DesD



- Molecule 1: desferrioxamine E biosynthesis protein DesD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.32Å 95.70Å 181.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.27 – 1.92 58.20 – 1.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.27-1.92) 100.0 (58.20-1.92)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.94 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.160 , 0.186 0.170 , 0.193	Depositor DCC
$R_{free}$ test set	4796 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8422e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.50	37/4828 (0.8%)	1.33	55/6572 (0.8%)
1	B	1.47	35/4825 (0.7%)	1.36	65/6568 (1.0%)
All	All	1.48	72/9653 (0.7%)	1.34	120/13140 (0.9%)

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CD-OE2	14.39	1.41	1.25
1	A	534	GLU	CD-OE2	11.85	1.38	1.25
1	A	272	GLU	CD-OE2	-10.22	1.14	1.25
1	A	355	GLU	CD-OE2	-10.19	1.14	1.25
1	B	205	GLU	CD-OE2	9.98	1.36	1.25
1	B	541	GLU	CD-OE2	9.68	1.36	1.25
1	B	272	GLU	CD-OE2	-8.94	1.15	1.25
1	B	374	GLU	CG-CD	8.77	1.65	1.51
1	A	206	TYR	CG-CD1	-8.70	1.27	1.39
1	B	416	GLU	CD-OE1	8.55	1.35	1.25
1	A	353	GLU	CD-OE1	-8.48	1.16	1.25
1	A	116	GLU	CB-CG	-8.26	1.36	1.52
1	A	534	GLU	CG-CD	8.20	1.64	1.51
1	A	205	GLU	CD-OE1	8.13	1.34	1.25
1	B	138	GLU	CD-OE1	7.89	1.34	1.25
1	A	312	TYR	CB-CG	-7.79	1.40	1.51
1	B	116	GLU	CB-CG	-7.76	1.37	1.52
1	B	416	GLU	CG-CD	7.70	1.63	1.51
1	A	416	GLU	CD-OE1	7.36	1.33	1.25
1	B	272	GLU	CD-OE1	-7.24	1.17	1.25
1	A	95	ASP	CG-OD2	-7.23	1.08	1.25
1	B	95	ASP	CG-OD2	-7.07	1.09	1.25
1	A	374	GLU	CB-CG	-7.05	1.38	1.52
1	B	374	GLU	CB-CG	-6.96	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLU	CG-CD	6.96	1.62	1.51
1	B	268	GLU	CD-OE2	-6.81	1.18	1.25
1	A	382	GLU	CD-OE2	6.75	1.33	1.25
1	A	541	GLU	CD-OE2	6.64	1.32	1.25
1	B	207	GLU	CD-OE1	6.62	1.32	1.25
1	B	120	SER	CB-OG	-6.62	1.33	1.42
1	A	432	SER	CA-CB	-6.48	1.43	1.52
1	A	535	TYR	CE1-CZ	6.41	1.46	1.38
1	B	229	ARG	CD-NE	6.39	1.57	1.46
1	A	374	GLU	CD-OE1	-6.17	1.18	1.25
1	A	272	GLU	CD-OE1	-6.15	1.18	1.25
1	A	117	GLU	CD-OE2	6.09	1.32	1.25
1	B	515	GLU	CD-OE1	6.09	1.32	1.25
1	A	116	GLU	CG-CD	6.06	1.61	1.51
1	A	353	GLU	CD-OE2	-5.90	1.19	1.25
1	B	515	GLU	CG-CD	5.88	1.60	1.51
1	B	335	GLU	CD-OE1	5.86	1.32	1.25
1	A	541	GLU	CG-CD	5.83	1.60	1.51
1	A	445	GLU	CB-CG	-5.81	1.41	1.52
1	B	138	GLU	CD-OE2	5.78	1.32	1.25
1	B	116	GLU	CG-CD	5.77	1.60	1.51
1	B	445	GLU	CB-CG	-5.75	1.41	1.52
1	A	515	GLU	CD-OE1	5.73	1.31	1.25
1	A	268	GLU	CB-CG	-5.69	1.41	1.52
1	A	374	GLU	CD-OE2	-5.50	1.19	1.25
1	B	133	GLN	CD-NE2	5.49	1.46	1.32
1	B	534	GLU	CD-OE2	5.47	1.31	1.25
1	A	374	GLU	CG-CD	5.46	1.60	1.51
1	A	268	GLU	CD-OE2	-5.46	1.19	1.25
1	A	354	TYR	CB-CG	5.46	1.59	1.51
1	B	521	GLU	CD-OE1	5.41	1.31	1.25
1	B	123[A]	SER	CB-OG	-5.34	1.35	1.42
1	B	123[B]	SER	CB-OG	-5.34	1.35	1.42
1	B	354	TYR	CZ-OH	5.30	1.46	1.37
1	B	207	GLU	CG-CD	5.27	1.59	1.51
1	B	314	GLU	C-O	-5.27	1.13	1.23
1	A	416	GLU	CD-OE2	5.26	1.31	1.25
1	A	17	GLU	CD-OE2	5.26	1.31	1.25
1	B	17	GLU	CD-OE2	5.22	1.31	1.25
1	B	500	ASP	CG-OD2	-5.22	1.13	1.25
1	A	175	SER	CB-OG	-5.19	1.35	1.42
1	A	123	SER	CB-OG	-5.16	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	547	GLU	CD-OE2	5.14	1.31	1.25
1	A	445	GLU	CG-CD	5.09	1.59	1.51
1	B	312	TYR	CG-CD2	5.08	1.45	1.39
1	B	437	ASP	CB-CG	-5.06	1.41	1.51
1	A	109	GLU	CD-OE2	5.04	1.31	1.25
1	B	515	GLU	CD-OE2	5.02	1.31	1.25

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	ARG	NE-CZ-NH1	14.10	127.35	120.30
1	A	227	ARG	NE-CZ-NH2	-13.85	113.38	120.30
1	A	68	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	A	227	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	B	227	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	B	570	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	B	257	GLU	OE1-CD-OE2	-10.94	110.17	123.30
1	B	229	ARG	NE-CZ-NH2	10.57	125.59	120.30
1	A	344	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	570	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	A	359	ASP	CB-CG-OD2	-10.22	109.10	118.30
1	B	359	ASP	CB-CG-OD1	9.71	127.04	118.30
1	B	220	ASP	CB-CG-OD2	9.63	126.97	118.30
1	A	359	ASP	CB-CG-OD1	9.55	126.90	118.30
1	A	409	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	B	229	ARG	CG-CD-NE	8.99	130.69	111.80
1	B	211	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	195	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	B	71[A]	ASP	CB-CG-OD1	8.62	126.06	118.30
1	B	71[B]	ASP	CB-CG-OD1	8.62	126.06	118.30
1	B	211	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	B	20	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	B	354	TYR	CB-CG-CD1	8.18	125.91	121.00
1	A	419	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	68	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	548	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	354	TYR	CB-CG-CD1	7.44	125.47	121.00
1	A	272	GLU	OE1-CD-OE2	-7.35	114.47	123.30
1	A	592	LEU	CB-CG-CD1	7.33	123.47	111.00
1	A	71	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	526	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	534	GLU	CG-CD-OE1	-7.19	103.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	LEU	CB-CG-CD2	7.14	123.14	111.00
1	B	13	GLU	CG-CD-OE1	7.12	132.54	118.30
1	B	526	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	533	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	212	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	534	GLU	CG-CD-OE2	6.76	131.82	118.30
1	B	548	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	193	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	44	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	548	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	582	LEU	CB-CG-CD2	-6.61	99.77	111.00
1	A	168	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	B	344	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	56	ASP	CB-CG-OD1	6.46	124.12	118.30
1	B	56	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	462	LYS	CD-CE-NZ	6.45	126.53	111.70
1	B	76[A]	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	76[B]	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	168	PHE	CB-CG-CD1	6.38	125.26	120.80
1	B	116	GLU	CG-CD-OE1	-6.37	105.56	118.30
1	B	55	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	56	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	53	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	108	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	530	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	A	232	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	280	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	34	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	13	GLU	CG-CD-OE1	6.11	130.53	118.30
1	B	419	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	596	GLY	CA-C-O	-5.96	109.88	120.60
1	B	409	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	221	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	117	GLU	OE1-CD-OE2	5.83	130.30	123.30
1	A	211	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	270[A]	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	270[B]	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	441	MET	CG-SD-CE	5.80	109.49	100.20
1	A	350	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	419	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	570	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	43	ASP	CB-CG-OD1	5.75	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	LYS	CD-CE-NZ	5.74	124.91	111.70
1	B	13	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	B	592	LEU	CB-CG-CD1	5.74	120.75	111.00
1	A	299	VAL	CA-CB-CG1	5.73	119.50	110.90
1	A	457	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	94	LEU	CB-CG-CD2	5.65	120.61	111.00
1	A	211	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	48	GLN	N-CA-C	5.61	126.15	111.00
1	B	207	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	B	522	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	82	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	567	ARG	CG-CD-NE	5.49	123.32	111.80
1	A	20	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	461	TYR	CB-CG-CD1	5.47	124.28	121.00
1	B	416	GLU	CG-CD-OE1	5.47	129.24	118.30
1	A	589	LYS	CD-CE-NZ	-5.46	99.14	111.70
1	A	24	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	503	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	254	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	B	116	GLU	CG-CD-OE2	5.41	129.12	118.30
1	B	563	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	B	139	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	222	PHE	CB-CG-CD1	5.39	124.57	120.80
1	B	195	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	55	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	474	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	570	ARG	CB-CG-CD	5.32	125.43	111.60
1	A	453	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	271	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	349	TYR	CB-CG-CD1	5.25	124.15	121.00
1	B	170	ILE	CG1-CB-CG2	5.22	122.89	111.40
1	B	522	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	A	533	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	409	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	254	PHE	CB-CG-CD1	5.18	124.42	120.80
1	B	68	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	B	165	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	416	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	B	34	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	480	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	B	55	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	159	PHE	CB-CG-CD1	-5.06	117.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	30	PHE	CB-CG-CD1	5.04	124.33	120.80
1	B	229	ARG	CB-CG-CD	5.03	124.68	111.60
1	B	199	THR	CA-CB-CG2	-5.02	105.37	112.40
1	B	313	MET	CG-SD-CE	5.01	108.21	100.20

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	4704	0	4584	17	0
1	B	4701	0	4582	19	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	24	0	32	3	0
3	B	42	0	55	3	0
4	A	371	0	0	3	0
4	B	366	0	0	2	0
All	All	10211	0	9253	34	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 2.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:B:229:ARG:HB3	1:B:229:ARG:HH11	1.47	0.78
1:B:570:ARG:HH11	1:B:570:ARG:HB2	1.49	0.78
1:B:229:ARG:CB	1:B:229:ARG:HH11	2.11	0.63
1:A:156:HIS:HA	3:A:604:GOL:H32	1.83	0.60
1:A:229:ARG:HD2	4:A:902:HOH:O	2.01	0.59
1:B:229:ARG:HB3	1:B:229:ARG:NH1	2.17	0.58
1:B:43:ASP:HB2	1:B:47:GLY:N	2.22	0.54
1:A:416:GLU:HG2	4:A:1016:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:OG	1:A:138:GLU:HG3	2.08	0.53
1:B:567:ARG:HE	1:B:583:GLN:NE2	2.07	0.53
1:B:480:GLU:CD	1:B:480:GLU:H	2.14	0.51
1:A:41:GLU:OE2	1:A:62:ARG:NE	2.38	0.51
1:B:326:LEU:HD23	1:B:326:LEU:C	2.32	0.50
1:A:480:GLU:CD	1:A:480:GLU:H	2.15	0.49
1:B:156:HIS:HA	3:B:606:GOL:H32	1.95	0.48
1:B:571:GLN:HG3	1:B:573:VAL:O	2.13	0.48
1:B:583:GLN:OE1	4:B:701:HOH:O	2.20	0.48
1:A:571:GLN:HG3	1:A:573:VAL:O	2.14	0.48
1:A:371:LEU:C	1:A:371:LEU:HD12	2.34	0.47
1:B:41:GLU:OE2	1:B:62:ARG:NE	2.41	0.46
1:A:445:GLU:OE2	3:A:602:GOL:O2	2.33	0.46
1:B:371:LEU:HD12	1:B:371:LEU:C	2.36	0.46
1:A:15:TRP:CZ2	1:B:256:ALA:HB2	2.52	0.45
1:B:302:MET:CE	3:B:603:GOL:H32	2.48	0.44
1:A:312:TYR:CE1	1:A:483:ARG:HD3	2.52	0.44
1:A:326:LEU:HD23	1:A:326:LEU:C	2.38	0.43
1:A:270[A]:ASP:OD2	4:A:701:HOH:O	2.22	0.42
1:B:445:GLU:OE2	3:B:603:GOL:O2	2.37	0.42
1:A:391:SER:O	1:A:402:PHE:HB3	2.20	0.41
1:A:445:GLU:OE1	3:A:602:GOL:O3	2.35	0.41
1:A:112:PRO:HB2	1:B:364:TYR:CE2	2.55	0.41
1:B:409:ARG:NH1	4:B:712:HOH:O	2.44	0.41
1:B:338:LEU:HD22	1:B:428:PRO:HB3	2.02	0.41
1:A:498:PHE:O	1:A:502:PHE:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	595/594 (100%)	575 (97%)	19 (3%)	1 (0%)	47	38
1	B	595/594 (100%)	580 (98%)	15 (2%)	0	100	100
All	All	1190/1188 (100%)	1155 (97%)	34 (3%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLN

### 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	490/487 (101%)	480 (98%)	10 (2%)	55	49
1	B	490/487 (101%)	479 (98%)	11 (2%)	52	45
All	All	980/974 (101%)	959 (98%)	21 (2%)	52	46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	48	GLN
1	A	95	ASP
1	A	280	ARG
1	A	305	MET
1	A	443	HIS
1	A	481	VAL
1	A	515	GLU
1	A	534	GLU
1	A	570	ARG
1	B	43	ASP
1	B	48	GLN
1	B	49	THR
1	B	95	ASP
1	B	229	ARG

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Mol	Chain	Res	Type
1	B	280	ARG
1	B	443	HIS
1	B	481	VAL
1	B	483	ARG
1	B	515	GLU
1	B	570	ARG

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

Mol	Chain	Res	Type
1	A	163	ASN
1	A	443	HIS
1	B	48	GLN
1	B	163	ASN
1	B	583	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	603	-	5,5,5	0.60	0	5,5,5	1.97	2 (40%)
3	GOL	A	603	-	5,5,5	0.66	0	5,5,5	1.89	2 (40%)
3	GOL	B	607	-	5,5,5	1.08	0	5,5,5	1.13	0
3	GOL	B	609	-	5,5,5	0.70	0	5,5,5	1.50	2 (40%)
3	GOL	B	608	-	5,5,5	0.46	0	5,5,5	1.38	1 (20%)
3	GOL	A	604	-	5,5,5	0.53	0	5,5,5	0.90	0
3	GOL	B	606	-	5,5,5	0.63	0	5,5,5	1.34	0
3	GOL	B	605	-	5,5,5	0.81	0	5,5,5	1.18	1 (20%)
3	GOL	A	602	-	5,5,5	0.46	0	5,5,5	1.76	1 (20%)
3	GOL	A	605	-	5,5,5	0.81	0	5,5,5	1.81	1 (20%)
3	GOL	B	604	-	5,5,5	0.55	0	5,5,5	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	603	-	-	3/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	B	607	-	-	1/4/4/4	-
3	GOL	B	609	-	-	2/4/4/4	-
3	GOL	B	608	-	-	2/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	B	606	-	-	1/4/4/4	-
3	GOL	B	605	-	-	0/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	B	604	-	-	0/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	GOL	O3-C3-C2	-3.44	93.72	110.20
3	A	605	GOL	O2-C2-C1	3.34	123.85	109.12
3	B	603	GOL	C3-C2-C1	2.81	122.63	111.70
3	A	602	GOL	C3-C2-C1	2.66	122.04	111.70
3	B	609	GOL	O3-C3-C2	2.24	120.95	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	609	GOL	O2-C2-C1	2.14	118.55	109.12
3	B	605	GOL	C3-C2-C1	-2.12	103.45	111.70
3	A	603	GOL	O1-C1-C2	-2.07	100.26	110.20
3	B	608	GOL	O2-C2-C3	-2.06	100.03	109.12
3	B	603	GOL	O3-C3-C2	2.02	119.88	110.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	GOL	O1-C1-C2-C3
3	B	609	GOL	C1-C2-C3-O3
3	A	603	GOL	C1-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	A	605	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	B	609	GOL	O2-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	A	604	GOL	O1-C1-C2-C3
3	B	607	GOL	C1-C2-C3-O3
3	B	603	GOL	O2-C2-C3-O3
3	A	605	GOL	O2-C2-C3-O3
3	B	606	GOL	O1-C1-C2-C3
3	B	608	GOL	C1-C2-C3-O3
3	B	608	GOL	O2-C2-C3-O3
3	A	604	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	GOL	2	0
3	A	604	GOL	1	0
3	B	606	GOL	1	0
3	A	602	GOL	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<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	594/594 (100%)	-0.13	15 (2%) 57 60	9, 17, 41, 96	0
1	B	593/594 (99%)	-0.16	16 (2%) 54 57	9, 18, 41, 101	0
All	All	1187/1188 (99%)	-0.14	31 (2%) 56 59	9, 17, 41, 101	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	GLY	9.6
1	B	46	GLY	8.3
1	A	576	ALA	8.1
1	A	578	PRO	6.3
1	A	575	LEU	5.8
1	B	44	ASP	5.5
1	B	47	GLY	5.4
1	A	46	GLY	5.0
1	B	45	GLY	4.2
1	B	42	PRO	4.2
1	B	312	TYR	3.8
1	B	575	LEU	3.5
1	A	573	VAL	3.4
1	A	42	PRO	3.1
1	B	43	ASP	3.1
1	A	47	GLY	3.0
1	B	576	ALA	3.0
1	A	44	ASP	2.9
1	A	476	VAL	2.5
1	B	578	PRO	2.4
1	A	40	ARG	2.4
1	A	479	PRO	2.3
1	A	577	ASP	2.3
1	B	48	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	43	ASP	2.2
1	B	381	ARG	2.2
1	B	382	GLU	2.2
1	A	570	ARG	2.2
1	B	574	ASP	2.2
1	B	479	PRO	2.1
1	B	579	SER	2.1

## 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 carbohydrates 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
3	GOL	A	603	6/6	0.89	0.21	29,31,37,40	0
3	GOL	B	605	6/6	0.89	0.14	25,25,28,28	0
3	GOL	A	605	6/6	0.91	0.17	17,32,35,41	0
3	GOL	B	607	6/6	0.93	0.10	19,30,31,31	0
3	GOL	A	604	6/6	0.93	0.19	20,26,28,29	0
3	GOL	B	604	6/6	0.93	0.11	18,26,30,44	0
3	GOL	B	608	6/6	0.93	0.13	19,23,28,37	0
2	CL	B	602	1/1	0.94	0.07	28,28,28,28	0
3	GOL	B	609	6/6	0.94	0.18	15,29,30,31	0
3	GOL	B	603	6/6	0.94	0.14	17,19,22,23	0
3	GOL	A	602	6/6	0.95	0.15	21,24,28,29	0
3	GOL	B	606	6/6	0.98	0.17	20,20,24,25	0
2	CL	B	601	1/1	1.00	0.04	15,15,15,15	0
2	CL	A	601	1/1	1.00	0.05	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.