



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:53 AM GMT

PDB ID : 1RNR  
Title : AUTOCATALYTIC GENERATION OF DOPA IN THE ENGINEERED PROTEIN R2 F208Y FROM ESCHERICHIA COLI RIBONUCLEOTIDE REDUCTASE AND CRYSTAL STRUCTURE OF THE DOPA-208 PROTEIN  
Authors : Aberg, A.; Nordlund, P.  
Deposited on : 1993-04-26  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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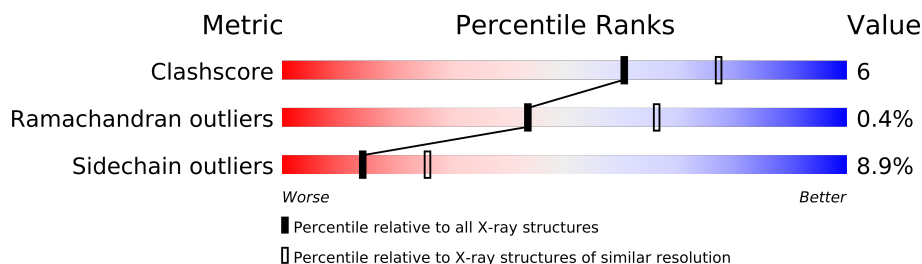
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5727 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2786	1782	463	528	13			
1	B	340	Total	C	N	O	S	0	0	0
			2786	1782	463	528	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	GLN	CONFLICT	UNP P69924
A	24	GLN	ASN	CONFLICT	UNP P69924
A	208	DAH	PHE	ENGINEERED MUTATION	UNP P69924
A	326	ASN	GLN	CONFLICT	UNP P69924
B	7	ALA	GLN	CONFLICT	UNP P69924
B	24	GLN	ASN	CONFLICT	UNP P69924
B	208	DAH	PHE	ENGINEERED MUTATION	UNP P69924
B	326	ASN	GLN	CONFLICT	UNP P69924

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	8	Total	Hg	0	0
			8	8		
3	A	6	Total	Hg	0	0
			6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	1	0
4	B	65	Total 65	O 65	1	0

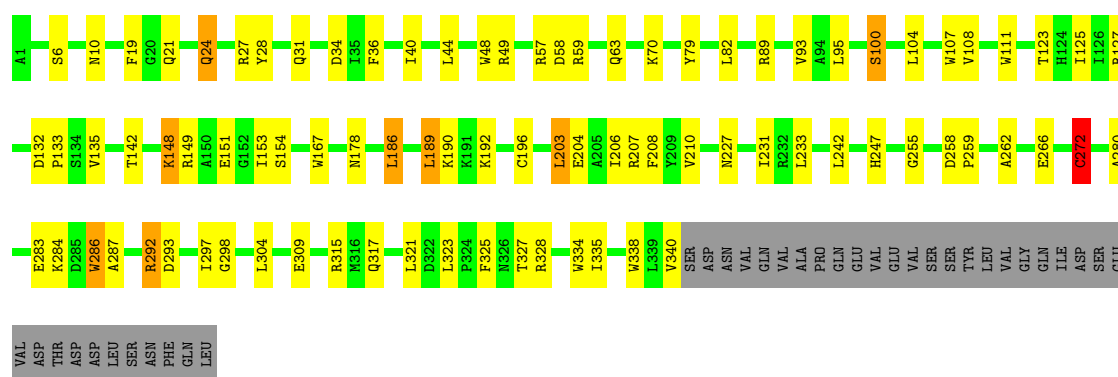
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

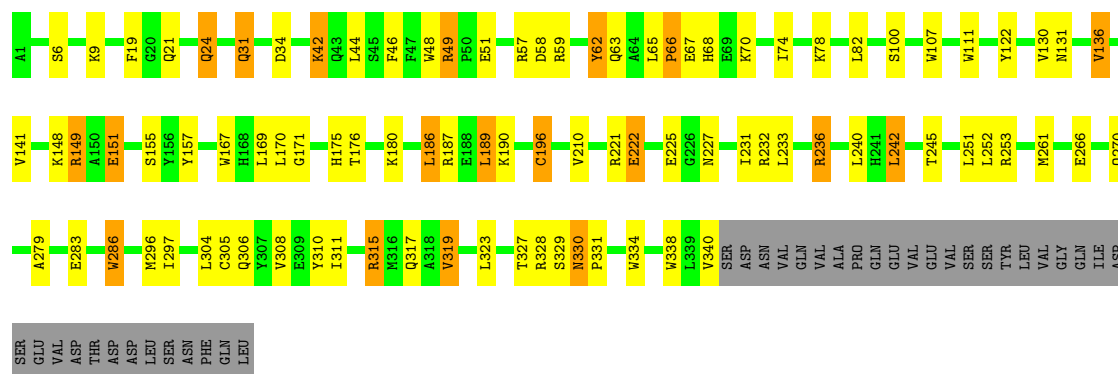
#### • Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain A:



#### • Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.10Å 85.30Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 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: DAH, FE, HG

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	0.82	1/2835 (0.0%)	1.55	48/3845 (1.2%)
1	B	0.80	0/2835	1.54	51/3845 (1.3%)
All	All	0.81	1/5670 (0.0%)	1.54	99/7690 (1.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	GLY	N-CA	6.76	1.56	1.46

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	B	286	TRP	CD1-CG-CD2	9.61	113.99	106.30
1	B	338	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	A	89	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	A	27	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	167	TRP	CD1-CG-CD2	8.68	113.25	106.30
1	A	28	TYR	CB-CG-CD2	-8.66	115.80	121.00
1	B	286	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	A	286	TRP	CE2-CD2-CG	-8.18	100.76	107.30
1	B	111	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	A	286	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	B	196	CYS	CA-CB-SG	-7.97	99.66	114.00
1	A	107	TRP	CE2-CD2-CG	-7.94	100.94	107.30
1	A	338	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	B	328	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	334	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	A	272	CYS	CA-CB-SG	7.83	128.09	114.00
1	B	48	TRP	CD1-CG-CD2	7.78	112.52	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	A	334	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	B	111	TRP	CE2-CD2-CG	-7.71	101.14	107.30
1	A	286	TRP	CG-CD2-CE3	7.64	140.78	133.90
1	B	334	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	B	338	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	334	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	B	107	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	A	338	TRP	CE2-CD2-CG	-7.51	101.30	107.30
1	B	296	MET	CG-SD-CE	-7.46	88.26	100.20
1	A	107	TRP	CD1-CG-CD2	7.42	112.23	106.30
1	B	157	TYR	CB-CG-CD1	-7.35	116.59	121.00
1	A	242	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	111	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	B	48	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	B	242	LEU	CA-CB-CG	7.03	131.46	115.30
1	A	59	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	111	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	B	232	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	107	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	B	149	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	B	107	TRP	CB-CG-CD1	-6.74	118.24	127.00
1	B	167	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	A	48	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	B	334	TRP	CG-CD2-CE3	6.64	139.87	133.90
1	B	338	TRP	CG-CD1-NE1	-6.55	103.55	110.10
1	B	167	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	B	59	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	48	TRP	CD1-CG-CD2	6.42	111.43	106.30
1	B	305	CYS	N-CA-CB	6.36	122.05	110.60
1	B	62	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	B	48	TRP	CB-CG-CD1	-6.26	118.87	127.00
1	B	107	TRP	CG-CD2-CE3	6.23	139.50	133.90
1	B	304	LEU	CA-C-N	6.22	130.89	117.20
1	B	310	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	167	TRP	CE2-CD2-CG	-6.11	102.41	107.30
1	A	328	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	122	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	A	27	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	328	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	286	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	A	315	ARG	NE-CZ-NH2	-5.91	117.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	111	TRP	CG-CD2-CE3	5.88	139.19	133.90
1	B	225	GLU	CA-C-N	5.85	127.89	116.20
1	A	334	TRP	CB-CG-CD1	-5.83	119.42	127.00
1	A	167	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	B	187	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	286	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	B	49	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	272	CYS	N-CA-CB	-5.71	100.32	110.60
1	A	207	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	334	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	B	319	VAL	CA-CB-CG2	-5.66	102.42	110.90
1	A	79	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	B	286	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	A	297	ILE	C-N-CA	-5.60	110.54	122.30
1	B	286	TRP	CB-CG-CD1	-5.59	119.73	127.00
1	B	236	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	319	VAL	N-CA-CB	-5.55	99.30	111.50
1	B	315	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	334	TRP	CB-CG-CD1	-5.50	119.85	127.00
1	A	108	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	B	111	TRP	CG-CD2-CE3	5.43	138.79	133.90
1	B	222	GLU	CA-CB-CG	5.43	125.34	113.40
1	B	111	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	A	49	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	93	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	247	HIS	CA-CB-CG	-5.31	104.58	113.60
1	B	319	VAL	CB-CA-C	5.30	121.47	111.40
1	B	319	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	A	242	LEU	N-CA-CB	-5.28	99.85	110.40
1	B	340	VAL	N-CA-C	-5.27	96.76	111.00
1	B	48	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	A	203	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	70	LYS	CB-CG-CD	-5.20	98.08	111.60
1	B	48	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	111	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	338	TRP	CB-CG-CD1	-5.04	120.45	127.00
1	A	107	TRP	CB-CG-CD1	-5.01	120.48	127.00
1	A	340	VAL	CG1-CB-CG2	-5.01	102.89	110.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2786	0	2727	31	0
1	B	2786	0	2725	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	2	0
3	B	8	0	0	1	0
4	A	72	0	0	1	0
4	B	65	0	0	1	0
All	All	5727	0	5452	57	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (57) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:CYS:HG	3:A:406:HG:HG	1.14	0.87
1:A:272:CYS:CB	3:A:407:HG:HG	1.84	0.85
1:A:272:CYS:SG	1:A:321:LEU:HD21	2.25	0.77
1:B:252:LEU:HD22	1:B:261:MET:HG2	1.69	0.75
1:A:266:GLU:HG2	4:A:480:HOH:O	1.87	0.74
1:A:123:THR:HG22	1:A:127:ARG:HH11	1.53	0.73
1:A:31:GLN:HG3	1:A:34:ASP:HA	1.80	0.64
1:B:42:LYS:HG2	1:B:240:LEU:HD21	1.80	0.63
1:A:309:GLU:HG3	1:A:325:PHE:CG	2.35	0.61
1:A:6:SER:O	1:A:24:GLN:HG2	2.01	0.60
1:B:6:SER:O	1:B:24:GLN:HG2	2.05	0.57
1:A:287:ALA:HB2	1:A:304:LEU:HD22	1.85	0.57
1:B:62:TYR:HA	1:B:65:LEU:HD22	1.87	0.56
1:A:149:ARG:HD2	1:A:286:TRP:CD2	2.42	0.55
1:B:317:GLN:HB2	1:B:323:LEU:HD21	1.88	0.54
1:B:329:SER:HB3	4:B:473:HOH:O	2.07	0.54
1:B:221:ARG:HD3	1:B:297:ILE:HD12	1.89	0.53
1:B:46:PHE:CD2	1:B:236:ARG:HD3	2.44	0.53
1:A:317:GLN:HB2	1:A:323:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:PHE:CE1	1:A:189:LEU:HD13	2.45	0.52
1:B:78:LYS:HG2	1:B:136:VAL:HG23	1.94	0.50
1:B:31:GLN:HG3	1:B:34:ASP:HA	1.94	0.50
1:B:311:ILE:O	1:B:315:ARG:HG2	2.11	0.50
1:A:255:GLY:HA2	1:A:262:ALA:HB2	1.95	0.49
1:A:19:PHE:HE1	1:A:189:LEU:HD13	1.77	0.49
1:A:125:ILE:HD13	1:A:227:ASN:HD22	1.78	0.48
1:B:196:CYS:HG	3:B:408:HG:HG	0.55	0.48
1:A:227:ASN:O	1:A:231:ILE:HG12	2.14	0.48
1:B:279:ALA:O	1:B:283:GLU:HG2	2.14	0.46
1:A:186:LEU:O	1:A:190:LYS:HG3	2.16	0.45
1:B:186:LEU:O	1:B:190:LYS:HG3	2.16	0.45
1:A:178:ASN:HD21	1:B:175:HIS:CD2	2.35	0.45
1:A:132:ASP:O	1:A:135:VAL:HG22	2.16	0.45
1:A:40:ILE:O	1:A:44:LEU:HG	2.16	0.45
1:B:66:PRO:O	1:B:68:HIS:N	2.49	0.45
1:A:204:GLU:HA	1:A:208:DAH:HD1	1.98	0.45
1:B:330:ASN:HD22	1:B:331:PRO:HD2	1.82	0.44
1:A:148:LYS:O	1:A:151:GLU:HG2	2.18	0.43
1:A:149:ARG:HD2	1:A:286:TRP:CG	2.53	0.43
1:A:24:GLN:NE2	1:B:141:VAL:HG21	2.33	0.43
1:B:62:TYR:O	1:B:70:LYS:HE3	2.18	0.43
1:B:227:ASN:O	1:B:231:ILE:HG12	2.19	0.43
1:A:258:ASP:HA	1:A:259:PRO:HD2	1.80	0.42
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.73	0.42
1:A:292:ARG:HD3	1:A:293:ASP:OD1	2.18	0.42
1:A:36:PHE:O	1:A:40:ILE:HG13	2.20	0.42
1:B:210:VAL:HG22	1:B:308:VAL:HG22	2.01	0.42
1:B:148:LYS:O	1:B:151:GLU:HB3	2.20	0.41
1:B:49:ARG:HB3	1:B:51:GLU:OE1	2.20	0.41
1:B:149:ARG:HD2	1:B:286:TRP:CG	2.55	0.41
1:B:171:GLY:O	1:B:175:HIS:HE1	2.02	0.41
1:A:206:ILE:O	1:A:210:VAL:HG23	2.20	0.41
1:A:280:ALA:O	1:A:284:LYS:HG3	2.21	0.41
1:B:19:PHE:HE1	1:B:189:LEU:HD13	1.85	0.41
1:B:317:GLN:HB2	1:B:323:LEU:CD2	2.51	0.40
1:B:176:THR:HA	1:B:180:LYS:O	2.20	0.40
1:A:21:GLN:O	1:A:100:SER:HB3	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	337/375 (90%)	331 (98%)	5 (2%)	1 (0%)	50	73
1	B	337/375 (90%)	329 (98%)	6 (2%)	2 (1%)	33	55
All	All	674/750 (90%)	660 (98%)	11 (2%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	GLU
1	B	66	PRO
1	A	153	ILE

### 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	305/338 (90%)	284 (93%)	21 (7%)	22	39
1	B	305/338 (90%)	272 (89%)	33 (11%)	9	17
All	All	610/676 (90%)	556 (91%)	54 (9%)	14	26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	24	GLN
1	A	58	ASP
1	A	63	GLN
1	A	82	LEU
1	A	95	LEU

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Mol	Chain	Res	Type
1	A	100	SER
1	A	104	LEU
1	A	133	PRO
1	A	142	THR
1	A	148	LYS
1	A	154	SER
1	A	186	LEU
1	A	189	LEU
1	A	192	LYS
1	A	203	LEU
1	A	233	LEU
1	A	272	CYS
1	A	283	GLU
1	A	292	ARG
1	A	327	THR
1	B	9	LYS
1	B	21	GLN
1	B	24	GLN
1	B	31	GLN
1	B	42	LYS
1	B	44	LEU
1	B	57	ARG
1	B	58	ASP
1	B	63	GLN
1	B	74	ILE
1	B	82	LEU
1	B	100	SER
1	B	130	VAL
1	B	131	ASN
1	B	136	VAL
1	B	151	GLU
1	B	155	SER
1	B	169	LEU
1	B	170	LEU
1	B	186	LEU
1	B	189	LEU
1	B	222	GLU
1	B	233	LEU
1	B	242	LEU
1	B	245	THR
1	B	251	LEU
1	B	253	ARG

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Mol	Chain	Res	Type
1	B	266	GLU
1	B	270	GLN
1	B	306	GLN
1	B	319	VAL
1	B	327	THR
1	B	330	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	87	GLN
1	A	227	ASN
1	B	10	ASN
1	B	31	GLN
1	B	63	GLN
1	B	131	ASN
1	B	168	HIS
1	B	175	HIS
1	B	201	ASN
1	B	250	ASN
1	B	330	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	DAH	A	208	1,2	13,13,14	4.81	1 (7%)	15,17,19	1.52	4 (26%)
1	DAH	B	208	1,2	13,13,14	4.76	1 (7%)	15,17,19	1.55	2 (13%)

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
1	DAH	A	208	1,2	-	0/4/6/8	0/1/1/1
1	DAH	B	208	1,2	-	0/4/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	DAH	O-C	17.06	1.23	1.11
1	B	208	DAH	O-C	16.91	1.23	1.11

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	DAH	C-CA-N	-4.50	109.34	113.83
1	A	208	DAH	C-CA-N	-3.06	110.77	113.83
1	A	208	DAH	CE2-CD2-CG	-2.43	117.82	120.78
1	A	208	DAH	CD1-CE1-CZ	-2.38	117.91	120.50
1	B	208	DAH	CG-CB-CA	2.28	119.79	114.42
1	A	208	DAH	CE1-CZ-CE2	2.21	122.64	119.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.