



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:25 PM GMT

PDB ID : 1CDE
Title : STRUCTURES OF APO AND COMPLEXED ESCHERICHIA COLI
GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE
Authors : Almassy, R.J.; Janson, C.A.; Kan, C.-C.; Hostomska, Z.
Deposited on : 1992-05-15
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

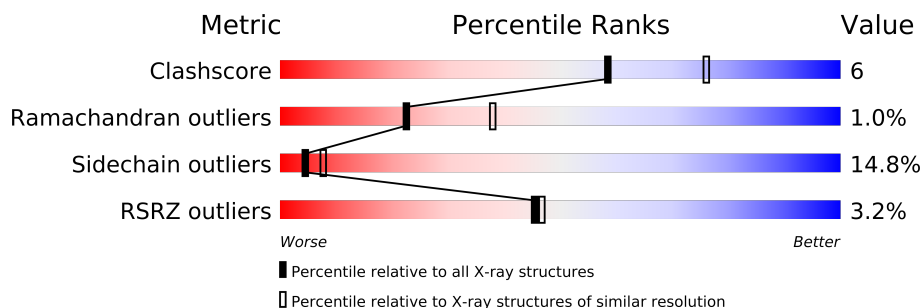
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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)
RSRZ outliers	66119	2785 (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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	
1	C	212	
1	D	212	

2 Entry composition i

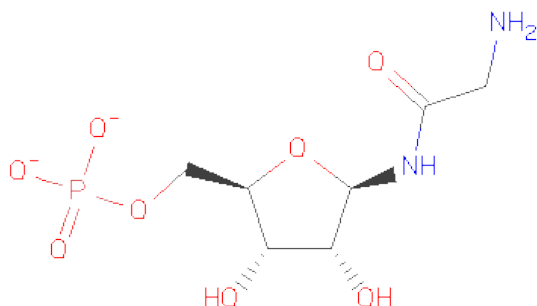
There are 3 unique types of molecules in this entry. The entry contains 6668 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHORIBOSYL-GLYCINAMIDEFORMYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	B	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	C	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	D	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			

- Molecule 2 is GLYCINAMIDE RIBONUCLEOTIDE (three-letter code: GAR) (formula: $C_7H_{13}N_2O_8P$).



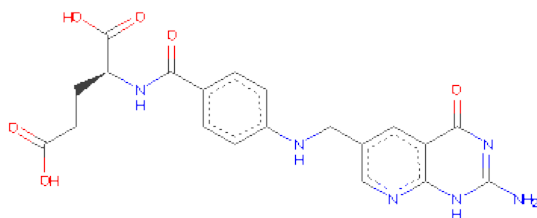
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			18	7	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			18	7	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			18	7	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			18	7	2	8	1		

- Molecule 3 is 5-DEAZAFOLIC ACID (three-letter code: DZF) (formula: $C_{20}H_{20}N_6O_6$).



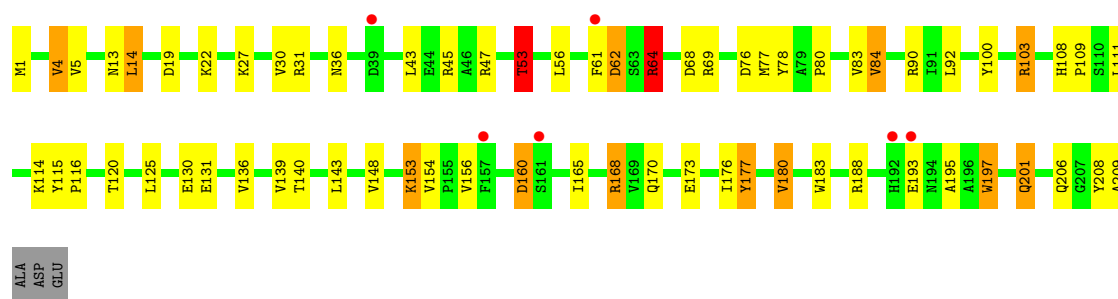
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	20	6	6		
3	B	1	Total	C	N	O	0	0
			32	20	6	6		
3	C	1	Total	C	N	O	0	0
			32	20	6	6		
3	D	1	Total	C	N	O	0	0
			32	20	6	6		

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.

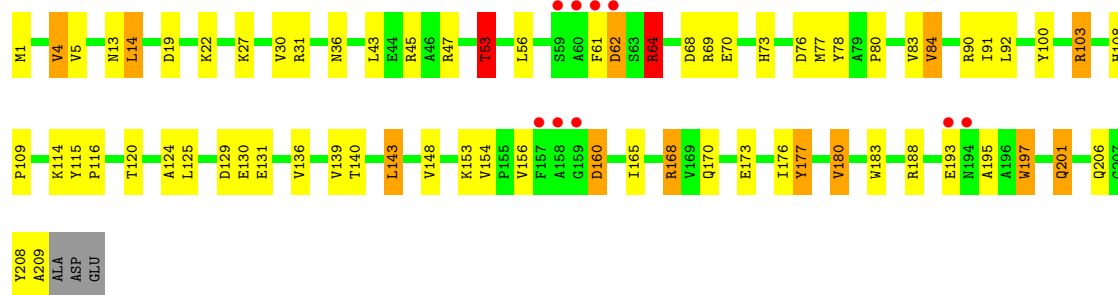
• Molecule 1: PHOSPHORIBOSYL-GLYCINAMIDEFORMYLTRANSFERASE

Chain A: 



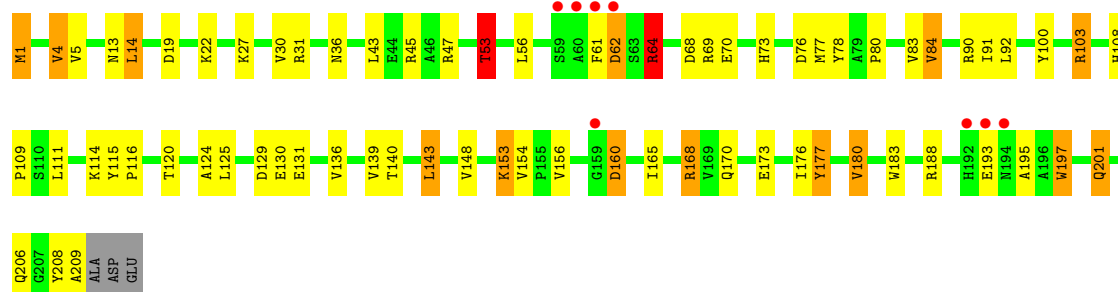
• Molecule 1: PHOSPHORIBOSYL-GLYCINAMIDEFORMYLTRANSFERASE

Chain B: 



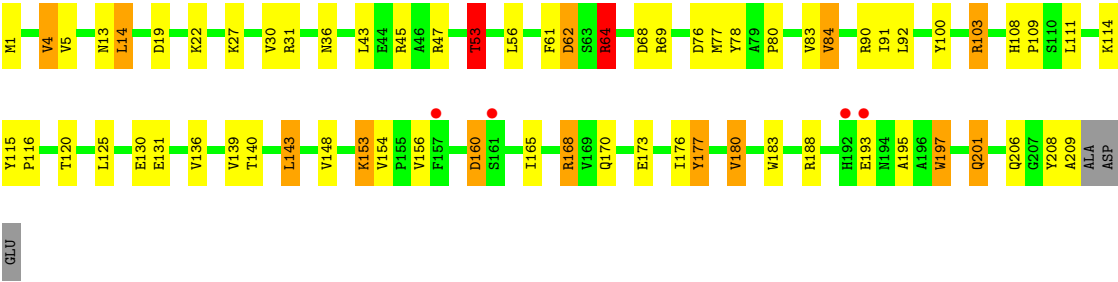
• Molecule 1: PHOSPHORIBOSYL-GLYCINAMIDEFORMYLTRANSFERASE

Chain C: 



● Molecule 1: PHOSPHORIBOSYL-GLYCINAMIDEFORMYLTRANSFERASE

Chain D:



GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.70Å 72.60Å 57.00Å 111.50° 82.80° 62.60°	Depositor
Resolution (Å)	(Not available) – 2.50 8.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 80.7 (8.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.52Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.250 , (Not available) 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25408 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6668	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAR, DZF

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	1.03	1/1654 (0.1%)	1.82	35/2248 (1.6%)
1	B	1.03	1/1654 (0.1%)	1.82	35/2248 (1.6%)
1	C	1.03	1/1654 (0.1%)	1.82	35/2248 (1.6%)
1	D	1.03	1/1654 (0.1%)	1.82	35/2248 (1.6%)
All	All	1.03	4/6616 (0.1%)	1.82	140/8992 (1.6%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	VAL	CA-CB	5.67	1.66	1.54
1	A	84	VAL	CA-CB	5.66	1.66	1.54
1	D	84	VAL	CA-CB	5.65	1.66	1.54
1	C	84	VAL	CA-CB	5.63	1.66	1.54

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ARG	NE-CZ-NH1	12.63	126.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	C	64	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	A	64	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	A	168	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	C	168	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	B	168	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	D	168	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	D	90	ARG	NE-CZ-NH2	-11.29	114.66	120.30
1	C	90	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	A	90	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	B	90	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	A	31	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	D	31	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	B	31	ARG	NE-CZ-NH2	-10.33	115.13	120.30
1	C	31	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	D	188	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	188	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	C	188	ARG	NE-CZ-NH2	-9.63	115.49	120.30
1	B	188	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	D	77	MET	CG-SD-CE	-8.53	86.55	100.20
1	A	77	MET	CG-SD-CE	-8.53	86.56	100.20
1	B	77	MET	CG-SD-CE	-8.53	86.56	100.20
1	C	77	MET	CG-SD-CE	-8.51	86.58	100.20
1	B	168	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	168	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	C	168	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	D	168	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	B	78	TYR	CB-CG-CD1	-8.06	116.16	121.00
1	A	78	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	D	78	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	C	78	TYR	CB-CG-CD1	-7.95	116.23	121.00
1	A	197	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	B	197	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	C	197	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	D	197	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	B	183	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	A	100	TYR	CB-CG-CD2	-7.44	116.54	121.00
1	B	100	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	A	183	TRP	CD1-CG-CD2	7.43	112.25	106.30
1	C	100	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	C	183	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	D	100	TYR	CB-CG-CD2	-7.42	116.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	TRP	CD1-CG-CD2	7.41	112.22	106.30
1	B	209	ALA	N-CA-CB	-7.38	99.78	110.10
1	A	209	ALA	N-CA-CB	-7.35	99.81	110.10
1	D	209	ALA	N-CA-CB	-7.35	99.81	110.10
1	C	209	ALA	N-CA-CB	-7.35	99.81	110.10
1	C	45	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	68	ASP	CB-CG-OD1	7.03	124.62	118.30
1	A	45	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	68	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	68	ASP	CB-CG-OD1	7.00	124.60	118.30
1	C	68	ASP	CB-CG-OD1	7.00	124.60	118.30
1	D	45	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	45	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	C	183	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	B	183	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	A	183	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	D	183	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	B	197	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	197	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	160	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	197	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	D	160	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	160	ASP	CB-CG-OD1	6.78	124.41	118.30
1	C	160	ASP	CB-CG-OD1	6.76	124.38	118.30
1	D	197	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	C	160	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	160	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	D	160	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	160	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	27	LYS	CA-CB-CG	6.42	127.52	113.40
1	A	27	LYS	CA-CB-CG	6.41	127.49	113.40
1	D	27	LYS	CA-CB-CG	6.40	127.49	113.40
1	B	27	LYS	CA-CB-CG	6.40	127.47	113.40
1	B	114	LYS	CA-C-N	6.38	131.23	117.20
1	A	114	LYS	CA-C-N	6.36	131.19	117.20
1	C	114	LYS	CA-C-N	6.36	131.18	117.20
1	C	131	GLU	N-CA-CB	-6.35	99.17	110.60
1	D	114	LYS	CA-C-N	6.35	131.16	117.20
1	D	131	GLU	N-CA-CB	-6.33	99.21	110.60
1	A	131	GLU	N-CA-CB	-6.33	99.21	110.60
1	B	131	GLU	N-CA-CB	-6.32	99.23	110.60
1	B	208	TYR	CA-C-N	-6.21	103.53	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	TYR	CA-C-N	-6.20	103.57	117.20
1	D	208	TYR	CA-C-N	-6.19	103.58	117.20
1	C	208	TYR	CA-C-N	-6.18	103.59	117.20
1	C	148	VAL	CG1-CB-CG2	-6.08	101.17	110.90
1	C	14	LEU	CA-CB-CG	6.08	129.28	115.30
1	D	148	VAL	CG1-CB-CG2	-6.07	101.19	110.90
1	B	14	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	14	LEU	CA-CB-CG	6.06	129.25	115.30
1	A	148	VAL	CG1-CB-CG2	-6.06	101.21	110.90
1	D	14	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	148	VAL	CG1-CB-CG2	-6.05	101.22	110.90
1	D	53	THR	CA-CB-CG2	6.02	120.83	112.40
1	C	90	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	53	THR	CA-CB-CG2	6.01	120.81	112.40
1	D	90	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	53	THR	CA-CB-OG1	-5.98	96.44	109.00
1	A	53	THR	CA-CB-CG2	5.98	120.77	112.40
1	A	53	THR	CA-CB-OG1	-5.98	96.45	109.00
1	B	53	THR	CA-CB-OG1	-5.98	96.45	109.00
1	B	53	THR	CA-CB-CG2	5.97	120.76	112.40
1	A	90	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	53	THR	CA-CB-OG1	-5.97	96.46	109.00
1	B	90	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	170	GLN	CA-CB-CG	-5.88	100.47	113.40
1	A	170	GLN	CA-CB-CG	-5.86	100.50	113.40
1	B	170	GLN	CA-CB-CG	-5.86	100.50	113.40
1	C	170	GLN	CA-CB-CG	-5.86	100.52	113.40
1	B	139	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	C	139	VAL	CG1-CB-CG2	-5.78	101.66	110.90
1	D	139	VAL	CG1-CB-CG2	-5.78	101.66	110.90
1	A	139	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	D	76	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	76	ASP	CB-CG-OD1	5.72	123.44	118.30
1	C	76	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	76	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	61	PHE	N-CA-C	5.41	125.59	111.00
1	B	61	PHE	N-CA-C	5.40	125.59	111.00
1	A	61	PHE	N-CA-C	5.39	125.56	111.00
1	C	61	PHE	N-CA-C	5.39	125.56	111.00
1	C	84	VAL	CG1-CB-CG2	-5.37	102.32	110.90
1	D	84	VAL	CG1-CB-CG2	-5.37	102.32	110.90
1	A	84	VAL	CG1-CB-CG2	-5.36	102.32	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	A	103	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	103	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	103	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	103	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	31	ARG	CG-CD-NE	5.17	122.66	111.80
1	A	31	ARG	CG-CD-NE	5.16	122.63	111.80
1	D	31	ARG	CG-CD-NE	5.16	122.63	111.80
1	C	31	ARG	CG-CD-NE	5.15	122.61	111.80
1	D	30	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	A	30	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	C	30	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	B	30	VAL	CG1-CB-CG2	-5.08	102.77	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	TYR	Sidechain
1	B	177	TYR	Sidechain
1	C	177	TYR	Sidechain
1	D	177	TYR	Sidechain

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	1617	0	1592	19	0
1	B	1617	0	1592	20	4
1	C	1617	0	1592	22	4
1	D	1617	0	1592	20	0
2	A	18	0	13	1	0
2	B	18	0	13	1	0
2	C	18	0	13	1	0
2	D	18	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	19	1	0
3	B	32	0	19	1	0
3	C	32	0	19	1	0
3	D	32	0	19	1	0
All	All	6668	0	6496	81	4

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:LEU:HD13	1:B:165:ILE:HD11	1.61	0.83
1:C:125:LEU:HD13	1:C:165:ILE:HD11	1.61	0.83
1:A:125:LEU:HD13	1:A:165:ILE:HD11	1.61	0.82
1:D:125:LEU:HD13	1:D:165:ILE:HD11	1.61	0.81
1:A:4:VAL:HG13	1:A:80:PRO:HB3	1.73	0.70
1:C:4:VAL:HG13	1:C:80:PRO:HB3	1.73	0.69
1:B:4:VAL:HG13	1:B:80:PRO:HB3	1.73	0.69
1:D:4:VAL:HG13	1:D:80:PRO:HB3	1.73	0.69
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.59	0.68
1:D:64:ARG:HG2	1:D:64:ARG:HH11	1.59	0.68
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.59	0.68
1:C:64:ARG:HG2	1:C:64:ARG:HH11	1.59	0.66
1:A:13:ASN:HD21	1:A:173:GLU:HB3	1.62	0.64
1:C:13:ASN:HD21	1:C:173:GLU:HB3	1.62	0.64
1:D:13:ASN:HD21	1:D:173:GLU:HB3	1.62	0.64
1:B:13:ASN:HD21	1:B:173:GLU:HB3	1.62	0.64
1:A:92:LEU:H	3:A:225:DZF:HN1	1.50	0.59
1:C:92:LEU:H	3:C:225:DZF:HN1	1.50	0.59
1:B:92:LEU:H	3:B:225:DZF:HN1	1.50	0.58
1:D:92:LEU:H	3:D:225:DZF:HN1	1.51	0.56
1:D:108:HIS:HD2	2:D:222:GAR:H241	1.54	0.56
1:B:108:HIS:HD2	2:B:222:GAR:H241	1.54	0.55
1:A:108:HIS:HD2	2:A:222:GAR:H241	1.54	0.55
1:C:108:HIS:HD2	2:C:222:GAR:H241	1.54	0.55
1:B:19:ASP:HA	1:B:22:LYS:HE3	1.89	0.55
1:C:64:ARG:NH1	1:C:64:ARG:HG2	2.21	0.55
1:D:19:ASP:HA	1:D:22:LYS:HE3	1.89	0.54
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.21	0.54
1:C:19:ASP:HA	1:C:22:LYS:HE3	1.89	0.54
1:A:19:ASP:HA	1:A:22:LYS:HE3	1.89	0.54
1:D:64:ARG:HG2	1:D:64:ARG:NH1	2.21	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:154:VAL:HG13	1:B:168:ARG:HG2	1.93	0.50
1:D:154:VAL:HG13	1:D:168:ARG:HG2	1.93	0.50
1:C:154:VAL:HG13	1:C:168:ARG:HG2	1.93	0.50
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.21	0.50
1:B:108:HIS:HE1	1:B:115:TYR:O	1.95	0.49
1:A:108:HIS:HE1	1:A:115:TYR:O	1.95	0.49
1:C:108:HIS:HE1	1:C:115:TYR:O	1.95	0.49
1:D:108:HIS:HE1	1:D:115:TYR:O	1.95	0.49
1:B:108:HIS:CD2	1:B:109:PRO:HD2	2.49	0.48
1:A:154:VAL:HG13	1:A:168:ARG:HG2	1.93	0.48
1:B:115:TYR:O	1:B:120:THR:HG22	2.14	0.48
1:A:108:HIS:CD2	1:A:109:PRO:HD2	2.49	0.48
1:D:108:HIS:CD2	1:D:109:PRO:HD2	2.49	0.48
1:D:115:TYR:O	1:D:120:THR:HG22	2.14	0.48
1:C:115:TYR:O	1:C:120:THR:HG22	2.14	0.47
1:A:115:TYR:O	1:A:120:THR:HG22	2.14	0.47
1:C:108:HIS:CD2	1:C:109:PRO:HD2	2.49	0.47
1:C:1:MET:HB2	1:C:1:MET:HE2	1.74	0.46
1:A:195:ALA:HB3	1:A:197:TRP:HE1	1.82	0.45
1:A:125:LEU:HD13	1:A:165:ILE:CD1	2.41	0.45
1:C:195:ALA:HB3	1:C:197:TRP:HE1	1.82	0.45
1:B:195:ALA:HB3	1:B:197:TRP:HE1	1.82	0.45
1:B:125:LEU:HD13	1:B:165:ILE:CD1	2.41	0.44
1:C:125:LEU:HD13	1:C:165:ILE:CD1	2.41	0.44
1:D:195:ALA:HB3	1:D:197:TRP:HE1	1.82	0.44
1:B:136:VAL:HG23	1:B:176:ILE:HD12	2.00	0.44
1:D:136:VAL:HG23	1:D:176:ILE:HD12	2.00	0.44
1:D:125:LEU:HD13	1:D:165:ILE:CD1	2.41	0.43
1:C:136:VAL:HG23	1:C:176:ILE:HD12	2.00	0.43
1:A:201:GLN:O	1:A:201:GLN:HG2	2.19	0.43
1:D:201:GLN:O	1:D:201:GLN:HG2	2.19	0.43
1:A:47:ARG:HH21	1:A:53:THR:HG21	1.85	0.42
1:C:136:VAL:HG11	1:C:180:VAL:HG21	2.02	0.42
1:D:47:ARG:HH21	1:D:53:THR:HG21	1.84	0.42
1:A:136:VAL:HG23	1:A:176:ILE:HD12	2.00	0.42
1:B:136:VAL:HG11	1:B:180:VAL:HG21	2.02	0.41
1:A:136:VAL:HG11	1:A:180:VAL:HG21	2.02	0.41
1:D:91:ILE:HG12	1:D:143:LEU:HD21	2.02	0.41
1:B:201:GLN:O	1:B:201:GLN:HG2	2.19	0.41
1:C:47:ARG:HH21	1:C:53:THR:HG21	1.84	0.41
1:D:136:VAL:HG11	1:D:180:VAL:HG21	2.02	0.41
1:B:47:ARG:HH21	1:B:53:THR:HG21	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:ILE:HG12	1:B:143:LEU:HD21	2.02	0.41
1:C:124:ALA:HA	1:C:129:ASP:OD2	2.21	0.41
1:C:91:ILE:HG12	1:C:143:LEU:HD21	2.02	0.41
1:C:201:GLN:HG2	1:C:201:GLN:O	2.19	0.41
1:C:111:LEU:HD13	1:C:153:LYS:HE2	2.03	0.41
1:A:111:LEU:HD13	1:A:153:LYS:HE2	2.03	0.41
1:B:124:ALA:HA	1:B:129:ASP:OD2	2.21	0.40
1:D:111:LEU:HD13	1:D:153:LYS:HE2	2.03	0.40

All (4) 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	Distance(Å)	Clash(Å)
1:B:73:HIS:NE2	1:C:70:GLU:OE1[1_465]	1.80	0.40
1:B:70:GLU:OE1	1:C:73:HIS:NE2[1_465]	1.86	0.34
1:B:73:HIS:CE1	1:C:70:GLU:OE1[1_465]	1.96	0.24
1:B:70:GLU:OE1	1:C:73:HIS:CE1[1_465]	1.97	0.23

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	207/212 (98%)	194 (94%)	11 (5%)	2 (1%)	22	38
1	B	207/212 (98%)	194 (94%)	11 (5%)	2 (1%)	22	38
1	C	207/212 (98%)	194 (94%)	11 (5%)	2 (1%)	22	38
1	D	207/212 (98%)	194 (94%)	11 (5%)	2 (1%)	22	38
All	All	828/848 (98%)	776 (94%)	44 (5%)	8 (1%)	22	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	B	193	GLU
1	C	193	GLU

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Mol	Chain	Res	Type
1	D	193	GLU
1	A	62	ASP
1	B	62	ASP
1	C	62	ASP
1	D	62	ASP

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	169/171 (99%)	144 (85%)	25 (15%)	4	8
1	B	169/171 (99%)	144 (85%)	25 (15%)	4	8
1	C	169/171 (99%)	144 (85%)	25 (15%)	4	8
1	D	169/171 (99%)	144 (85%)	25 (15%)	4	8
All	All	676/684 (99%)	576 (85%)	100 (15%)	4	8

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	VAL
1	A	5	VAL
1	A	14	LEU
1	A	36	ASN
1	A	43	LEU
1	A	53	THR
1	A	56	LEU
1	A	62	ASP
1	A	64	ARG
1	A	69	ARG
1	A	83	VAL
1	A	84	VAL
1	A	103	ARG
1	A	116	PRO
1	A	130	GLU
1	A	140	THR

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Mol	Chain	Res	Type
1	A	143	LEU
1	A	153	LYS
1	A	156	VAL
1	A	160	ASP
1	A	177	TYR
1	A	180	VAL
1	A	201	GLN
1	A	206	GLN
1	B	1	MET
1	B	4	VAL
1	B	5	VAL
1	B	14	LEU
1	B	36	ASN
1	B	43	LEU
1	B	53	THR
1	B	56	LEU
1	B	62	ASP
1	B	64	ARG
1	B	69	ARG
1	B	83	VAL
1	B	84	VAL
1	B	103	ARG
1	B	116	PRO
1	B	130	GLU
1	B	140	THR
1	B	143	LEU
1	B	153	LYS
1	B	156	VAL
1	B	160	ASP
1	B	177	TYR
1	B	180	VAL
1	B	201	GLN
1	B	206	GLN
1	C	1	MET
1	C	4	VAL
1	C	5	VAL
1	C	14	LEU
1	C	36	ASN
1	C	43	LEU
1	C	53	THR
1	C	56	LEU
1	C	62	ASP

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Mol	Chain	Res	Type
1	C	64	ARG
1	C	69	ARG
1	C	83	VAL
1	C	84	VAL
1	C	103	ARG
1	C	116	PRO
1	C	130	GLU
1	C	140	THR
1	C	143	LEU
1	C	153	LYS
1	C	156	VAL
1	C	160	ASP
1	C	177	TYR
1	C	180	VAL
1	C	201	GLN
1	C	206	GLN
1	D	1	MET
1	D	4	VAL
1	D	5	VAL
1	D	14	LEU
1	D	36	ASN
1	D	43	LEU
1	D	53	THR
1	D	56	LEU
1	D	62	ASP
1	D	64	ARG
1	D	69	ARG
1	D	83	VAL
1	D	84	VAL
1	D	103	ARG
1	D	116	PRO
1	D	130	GLU
1	D	140	THR
1	D	143	LEU
1	D	153	LYS
1	D	156	VAL
1	D	160	ASP
1	D	177	TYR
1	D	180	VAL
1	D	201	GLN
1	D	206	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	36	ASN
1	A	108	HIS
1	A	127	ASN
1	A	174	HIS
1	B	13	ASN
1	B	36	ASN
1	B	108	HIS
1	B	127	ASN
1	B	174	HIS
1	C	13	ASN
1	C	36	ASN
1	C	108	HIS
1	C	127	ASN
1	C	174	HIS
1	D	13	ASN
1	D	36	ASN
1	D	108	HIS
1	D	127	ASN
1	D	174	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	GAR	A	222	-	18,18,18	2.71	5 (27%)	26,26,26	1.82	8 (30%)
3	DZF	A	225	-	34,34,34	2.95	11 (32%)	45,47,47	2.84	14 (31%)
2	GAR	B	222	-	18,18,18	2.72	5 (27%)	26,26,26	1.81	8 (30%)
3	DZF	B	225	-	34,34,34	2.96	11 (32%)	45,47,47	2.84	14 (31%)
2	GAR	C	222	-	18,18,18	2.71	5 (27%)	26,26,26	1.81	8 (30%)
3	DZF	C	225	-	34,34,34	2.96	11 (32%)	45,47,47	2.84	14 (31%)
2	GAR	D	222	-	18,18,18	2.71	5 (27%)	26,26,26	1.82	8 (30%)
3	DZF	D	225	-	34,34,34	2.95	11 (32%)	45,47,47	2.84	14 (31%)

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	GAR	A	222	-	-	0/12/28/28	0/1/1/1
3	DZF	A	225	-	-	0/22/22/22	0/1/3/3
2	GAR	B	222	-	-	0/12/28/28	0/1/1/1
3	DZF	B	225	-	-	0/22/22/22	0/1/3/3
2	GAR	C	222	-	-	0/12/28/28	0/1/1/1
3	DZF	C	225	-	-	0/22/22/22	0/1/3/3
2	GAR	D	222	-	-	0/12/28/28	0/1/1/1
3	DZF	D	225	-	-	0/22/22/22	0/1/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	225	DZF	C7-C6	9.30	1.53	1.38
3	B	225	DZF	C7-C6	9.30	1.53	1.38
3	A	225	DZF	C7-C6	9.30	1.53	1.38
3	D	225	DZF	C7-C6	9.27	1.53	1.38
3	C	225	DZF	C7-N8	9.15	1.48	1.31
3	A	225	DZF	C7-N8	9.15	1.48	1.31
3	B	225	DZF	C7-N8	9.15	1.48	1.31
3	D	225	DZF	C7-N8	9.14	1.48	1.31
2	B	222	GAR	P15-O18	-6.98	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	222	GAR	P15-O18	-6.98	1.40	1.51
2	A	222	GAR	P15-O18	-6.97	1.40	1.51
2	D	222	GAR	P15-O18	-6.97	1.40	1.51
2	B	222	GAR	C3-N19	6.50	1.50	1.43
2	D	222	GAR	C3-N19	6.50	1.50	1.43
2	A	222	GAR	C3-N19	6.49	1.50	1.43
3	B	225	DZF	C5-C6	6.47	1.51	1.37
2	C	222	GAR	C3-N19	6.46	1.50	1.43
3	A	225	DZF	C5-C6	6.45	1.51	1.37
3	C	225	DZF	C5-C6	6.45	1.51	1.37
3	D	225	DZF	C5-C6	6.43	1.51	1.37
3	D	225	DZF	C8A-N1	-5.01	1.31	1.37
3	C	225	DZF	C8A-N1	-4.95	1.31	1.37
3	A	225	DZF	C8A-N1	-4.94	1.31	1.37
3	B	225	DZF	C8A-N1	-4.91	1.31	1.37
2	D	222	GAR	P15-O17	4.33	1.59	1.51
2	A	222	GAR	P15-O17	4.33	1.59	1.51
2	B	222	GAR	P15-O17	4.33	1.59	1.51
2	C	222	GAR	P15-O17	4.32	1.59	1.51
2	B	222	GAR	P15-O16	3.50	1.58	1.51
2	A	222	GAR	P15-O16	3.48	1.58	1.51
2	C	222	GAR	P15-O16	3.46	1.58	1.51
2	D	222	GAR	P15-O16	3.45	1.58	1.51
3	B	225	DZF	C4-N3	-3.04	1.31	1.37
3	A	225	DZF	C4-N3	-3.02	1.31	1.37
3	D	225	DZF	C4-N3	-3.00	1.31	1.37
3	C	225	DZF	C4-N3	-3.00	1.31	1.37
3	C	225	DZF	CB-CA	2.94	1.60	1.53
3	A	225	DZF	CB-CA	2.94	1.60	1.53
3	D	225	DZF	CB-CA	2.93	1.60	1.53
3	B	225	DZF	CB-CA	2.93	1.60	1.53
3	B	225	DZF	C8A-N8	-2.52	1.31	1.34
3	A	225	DZF	C8A-N8	-2.49	1.31	1.34
3	D	225	DZF	C8A-N8	-2.47	1.31	1.34
3	C	225	DZF	C8A-N8	-2.47	1.31	1.34
3	B	225	DZF	C4A-C8A	-2.41	1.37	1.41
3	C	225	DZF	C4A-C8A	-2.38	1.37	1.41
3	D	225	DZF	C2-N3	-2.36	1.30	1.33
3	C	225	DZF	C2-N3	-2.35	1.30	1.33
3	A	225	DZF	C4A-C8A	-2.34	1.37	1.41
3	A	225	DZF	C2-N3	-2.31	1.30	1.33
3	D	225	DZF	C11-C	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	225	DZF	C2-N3	-2.30	1.30	1.33
3	D	225	DZF	C4A-C8A	-2.28	1.38	1.41
3	C	225	DZF	C11-C	-2.28	1.45	1.50
3	A	225	DZF	C11-C	-2.27	1.45	1.50
3	B	225	DZF	C11-C	-2.24	1.45	1.50
2	B	222	GAR	P15-O12	-2.21	1.55	1.61
2	D	222	GAR	P15-O12	-2.20	1.55	1.61
2	A	222	GAR	P15-O12	-2.19	1.55	1.61
2	C	222	GAR	P15-O12	-2.18	1.55	1.61
3	A	225	DZF	O2-CT	2.12	1.37	1.30
3	D	225	DZF	O2-CT	2.12	1.37	1.30
3	C	225	DZF	O2-CT	2.12	1.37	1.30
3	B	225	DZF	O2-CT	2.12	1.37	1.30

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	225	DZF	C9-C6-C5	-11.03	105.18	122.27
3	B	225	DZF	C9-C6-C5	-11.02	105.19	122.27
3	A	225	DZF	C9-C6-C5	-11.01	105.20	122.27
3	D	225	DZF	C9-C6-C5	-11.00	105.22	122.27
3	C	225	DZF	C6-C7-N8	-7.25	110.96	123.73
3	B	225	DZF	C6-C7-N8	-7.22	111.00	123.73
3	A	225	DZF	C6-C7-N8	-7.22	111.02	123.73
3	D	225	DZF	C6-C7-N8	-7.19	111.06	123.73
3	A	225	DZF	C6-C9-N10	-5.42	101.64	113.73
3	B	225	DZF	C6-C9-N10	-5.42	101.65	113.73
3	D	225	DZF	C6-C9-N10	-5.42	101.65	113.73
3	C	225	DZF	C6-C9-N10	-5.41	101.66	113.73
3	D	225	DZF	CG-CB-CA	5.05	122.90	112.99
3	A	225	DZF	CG-CB-CA	5.04	122.88	112.99
3	B	225	DZF	CG-CB-CA	5.04	122.88	112.99
3	C	225	DZF	CG-CB-CA	5.02	122.83	112.99
2	A	222	GAR	O4-C3-C2	-4.69	100.82	105.99
2	D	222	GAR	O4-C3-C2	-4.68	100.83	105.99
2	C	222	GAR	O4-C3-C2	-4.68	100.83	105.99
2	B	222	GAR	O4-C3-C2	-4.66	100.85	105.99
3	C	225	DZF	C7-N8-C8A	4.29	122.71	116.62
3	B	225	DZF	C7-N8-C8A	4.29	122.71	116.62
3	D	225	DZF	C7-N8-C8A	4.29	122.71	116.62
3	A	225	DZF	C7-N8-C8A	4.28	122.70	116.62
3	C	225	DZF	C6-C5-C4A	-4.15	112.94	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	225	DZF	C6-C5-C4A	-4.15	112.96	122.10
3	A	225	DZF	C6-C5-C4A	-4.14	112.97	122.10
3	D	225	DZF	C6-C5-C4A	-4.13	112.99	122.10
2	C	222	GAR	C21-C23-N24	3.91	120.78	112.55
2	A	222	GAR	C21-C23-N24	3.91	120.78	112.55
2	D	222	GAR	C21-C23-N24	3.90	120.75	112.55
2	B	222	GAR	C21-C23-N24	3.89	120.74	112.55
3	B	225	DZF	C4A-C4-N3	-3.89	119.17	123.72
3	C	225	DZF	C4A-C4-N3	-3.86	119.21	123.72
3	A	225	DZF	C4A-C4-N3	-3.85	119.22	123.72
3	D	225	DZF	C4A-C4-N3	-3.81	119.26	123.72
3	B	225	DZF	C4-N3-C2	3.07	120.22	116.91
3	C	225	DZF	C4-N3-C2	3.03	120.19	116.91
3	A	225	DZF	C4-N3-C2	3.02	120.18	116.91
3	D	225	DZF	C4-N3-C2	3.01	120.16	116.91
3	D	225	DZF	O-C-C11	3.00	126.28	121.01
3	A	225	DZF	O-C-C11	2.99	126.26	121.01
3	C	225	DZF	O-C-C11	2.98	126.24	121.01
3	B	225	DZF	O-C-C11	2.97	126.22	121.01
3	B	225	DZF	C5-C4A-C8A	2.72	121.16	116.65
3	C	225	DZF	C5-C4A-C8A	2.71	121.15	116.65
3	D	225	DZF	C5-C4A-C8A	2.70	121.14	116.65
3	A	225	DZF	C5-C4A-C8A	2.70	121.13	116.65
3	C	225	DZF	C15-C14-N10	-2.59	115.74	121.02
3	D	225	DZF	C15-C14-N10	-2.57	115.76	121.02
3	B	225	DZF	C15-C14-N10	-2.57	115.77	121.02
3	A	225	DZF	C15-C14-N10	-2.57	115.77	121.02
3	B	225	DZF	C5-C6-C7	-2.52	114.06	116.66
3	D	225	DZF	C5-C6-C7	-2.52	114.06	116.66
3	A	225	DZF	C5-C6-C7	-2.50	114.08	116.66
3	D	225	DZF	C9-C6-C7	-2.48	114.27	120.71
3	A	225	DZF	C9-C6-C7	-2.48	114.28	120.71
3	C	225	DZF	C9-C6-C7	-2.47	114.30	120.71
3	B	225	DZF	C9-C6-C7	-2.46	114.32	120.71
3	C	225	DZF	C5-C6-C7	-2.44	114.14	116.66
2	A	222	GAR	O12-P15-O16	-2.40	99.31	105.86
2	B	222	GAR	O12-P15-O16	-2.39	99.31	105.86
2	D	222	GAR	C3-N19-C21	2.40	126.60	122.57
2	D	222	GAR	O12-P15-O16	-2.40	99.31	105.86
2	C	222	GAR	O12-P15-O16	-2.39	99.33	105.86
2	A	222	GAR	C3-N19-C21	2.39	126.59	122.57
2	C	222	GAR	C3-N19-C21	2.38	126.58	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	GAR	C3-N19-C21	2.37	126.56	122.57
2	D	222	GAR	C23-C21-N19	2.32	119.35	114.98
2	A	222	GAR	C23-C21-N19	2.31	119.33	114.98
2	C	222	GAR	C23-C21-N19	2.30	119.31	114.98
2	B	222	GAR	C23-C21-N19	2.28	119.28	114.98
3	D	225	DZF	CA-N-C	2.28	126.88	121.80
3	B	225	DZF	CA-N-C	2.27	126.86	121.80
3	A	225	DZF	CA-N-C	2.26	126.85	121.80
3	C	225	DZF	CA-N-C	2.25	126.82	121.80
2	B	222	GAR	C2-C3-N19	2.22	115.56	112.35
2	A	222	GAR	C2-C3-N19	2.22	115.55	112.35
2	D	222	GAR	C2-C3-N19	2.21	115.54	112.35
2	C	222	GAR	C2-C3-N19	2.20	115.53	112.35
2	B	222	GAR	O18-P15-O12	2.17	112.42	105.93
2	C	222	GAR	O18-P15-O12	2.15	112.37	105.93
2	A	222	GAR	O18-P15-O12	2.15	112.37	105.93
2	D	222	GAR	O18-P15-O12	2.14	112.34	105.93
2	D	222	GAR	C1-C2-C3	2.13	105.58	101.35
2	A	222	GAR	C1-C2-C3	2.13	105.57	101.35
2	C	222	GAR	C1-C2-C3	2.12	105.56	101.35
2	B	222	GAR	C1-C2-C3	2.12	105.55	101.35

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 ⓘ

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, 95th 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	209/212 (98%)	-0.16	6 (2%)	49	51	2, 19, 59, 86	0
1	B	209/212 (98%)	-0.12	9 (4%)	34	35	2, 19, 59, 86	0
1	C	209/212 (98%)	-0.12	8 (3%)	38	40	2, 19, 59, 86	0
1	D	209/212 (98%)	-0.25	4 (1%)	64	66	2, 19, 59, 86	0
All	All	836/848 (98%)	-0.16	27 (3%)	45	47	2, 20, 60, 86	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ALA	9.0
1	C	62	ASP	5.7
1	B	62	ASP	5.7
1	C	59	SER	5.5
1	C	60	ALA	5.0
1	C	192	HIS	4.6
1	A	161	SER	4.0
1	B	61	PHE	4.0
1	B	157	PHE	3.6
1	B	193	GLU	3.5
1	D	193	GLU	3.4
1	C	61	PHE	3.3
1	A	193	GLU	3.1
1	C	193	GLU	3.1
1	A	157	PHE	3.0
1	B	59	SER	3.0
1	B	194	ASN	2.8
1	C	194	ASN	2.7
1	B	159	GLY	2.6
1	C	159	GLY	2.5
1	A	192	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	157	PHE	2.4
1	A	39	ASP	2.4
1	B	158	ALA	2.3
1	D	161	SER	2.3
1	A	61	PHE	2.2
1	D	192	HIS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GAR	A	222	18/18	0.17	1.71	16,23,36,44	0
2	GAR	B	222	18/18	0.15	1.20	16,23,36,44	0
3	DZF	C	225	32/32	0.20	1.02	13,56,102,106	0
3	DZF	D	225	32/32	0.19	0.67	13,56,102,106	0
2	GAR	C	222	18/18	0.14	0.67	16,23,36,44	0
3	DZF	B	225	32/32	0.18	0.63	13,56,102,106	0
3	DZF	A	225	32/32	0.17	0.49	13,56,102,106	0
2	GAR	D	222	18/18	0.10	-0.46	16,23,36,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.