



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 PM UTC

PDB ID : 4UBR / pdb_00004ubr
Title : Crystal structure of Pseudomonas aeruginosa N-acetyltransferase PA4534
Authors : Choe, J.; Shin, S.
Deposited on : 2014-08-13
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

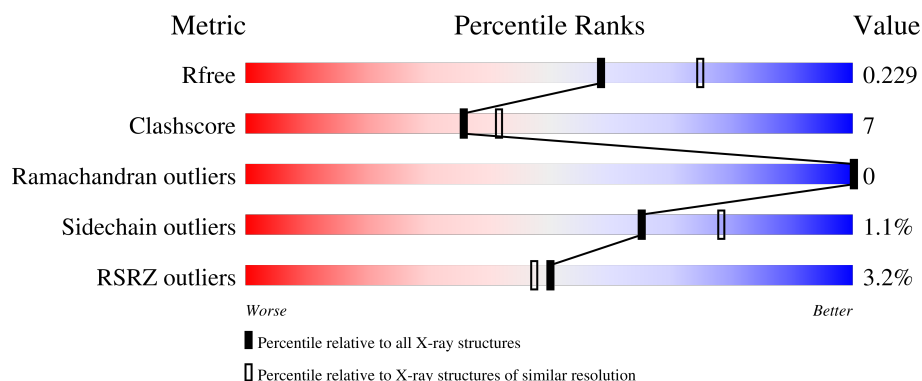
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	141	82% 15% .
1	B	141	84% 13% .
1	C	141	3% 85% 12% .
1	D	141	86% 11% .
1	E	141	87% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	141	
1	G	141	
1	H	141	
1	I	141	

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	GOL	D	201	-	-	X	-
2	GOL	F	201	-	-	X	-
2	GOL	F	202	-	-	X	-
2	GOL	G	201	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10510 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 Putative acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	B	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	C	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	D	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	E	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	F	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	G	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	H	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			
1	I	137	Total	C	N	O	S	0	0	0
			1095	695	205	191	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	VAL	ILE	conflict	UNP M1Y000
B	133	VAL	ILE	conflict	UNP M1Y000
C	133	VAL	ILE	conflict	UNP M1Y000
D	133	VAL	ILE	conflict	UNP M1Y000
E	133	VAL	ILE	conflict	UNP M1Y000
F	133	VAL	ILE	conflict	UNP M1Y000
G	133	VAL	ILE	conflict	UNP M1Y000
H	133	VAL	ILE	conflict	UNP M1Y000
I	133	VAL	ILE	conflict	UNP M1Y000

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		

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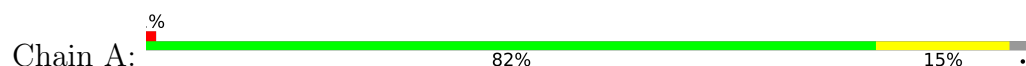
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	83	Total 83	O 83	0	0
3	C	72	Total 72	O 72	0	0
3	D	56	Total 56	O 56	0	0
3	E	81	Total 81	O 81	0	0
3	F	69	Total 69	O 69	0	0
3	G	53	Total 53	O 53	0	0
3	H	59	Total 59	O 59	0	0
3	I	51	Total 51	O 51	0	0

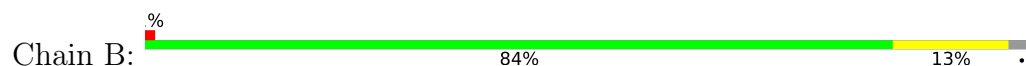
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

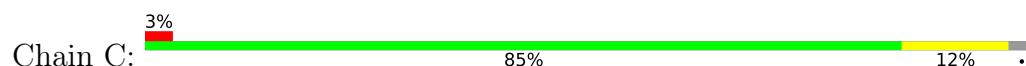
- Molecule 1: Putative acetyltransferase



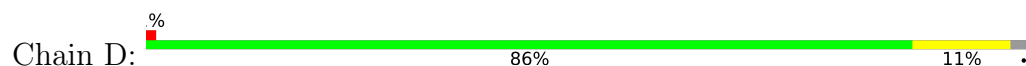
- Molecule 1: Putative acetyltransferase



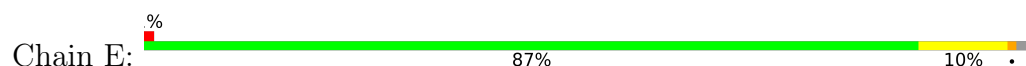
- Molecule 1: Putative acetyltransferase



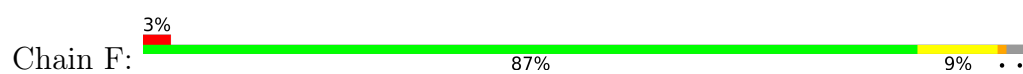
- Molecule 1: Putative acetyltransferase



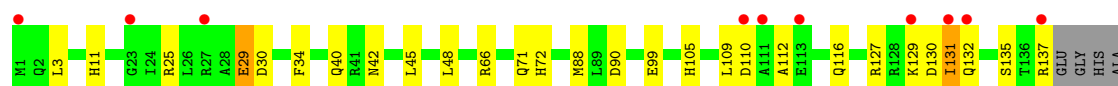
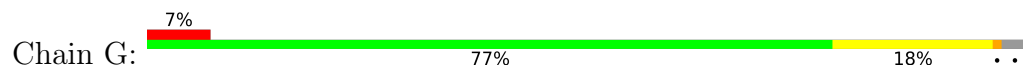
- Molecule 1: Putative acetyltransferase



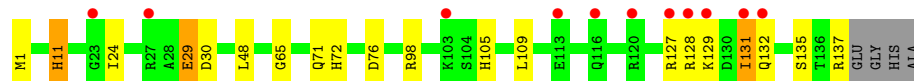
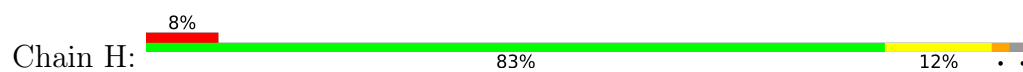
- Molecule 1: Putative acetyltransferase



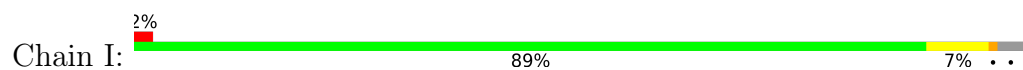
- Molecule 1: Putative acetyltransferase



- Molecule 1: Putative acetyltransferase



- Molecule 1: Putative acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.37Å 137.37Å 200.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.70 – 2.21 24.70 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.70-2.21) 99.7 (24.70-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192 , 0.228 0.199 , 0.229	Depositor DCC
R_{free} test set	4806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10510	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.11	0/1119	1.08	3/1512 (0.2%)
1	B	1.15	2/1119 (0.2%)	1.01	0/1512
1	C	1.14	1/1119 (0.1%)	1.08	0/1512
1	D	1.07	0/1119	0.99	2/1512 (0.1%)
1	E	1.17	1/1119 (0.1%)	1.07	2/1512 (0.1%)
1	F	1.05	1/1119 (0.1%)	1.05	2/1512 (0.1%)
1	G	1.19	0/1119	1.12	4/1512 (0.3%)
1	H	1.15	1/1119 (0.1%)	1.15	7/1512 (0.5%)
1	I	0.99	1/1119 (0.1%)	0.96	0/1512
All	All	1.11	7/10071 (0.1%)	1.06	20/13608 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	36	LEU	C-O	-7.39	1.15	1.24
1	C	32	TYR	C-O	-6.72	1.18	1.24
1	I	72	HIS	N-CA	5.91	1.53	1.46
1	E	63	HIS	CA-C	-5.64	1.45	1.52
1	H	128	ARG	CA-C	-5.35	1.46	1.52
1	B	90	ASP	C-O	-5.06	1.18	1.24
1	B	58	CYS	CA-C	-5.01	1.46	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	131	ILE	N-CA-C	8.10	120.53	108.46
1	H	131	ILE	N-CA-C	6.61	117.56	107.77
1	E	71	GLN	N-CA-C	6.45	120.82	111.02
1	H	65	GLY	N-CA-C	-6.41	106.47	115.32
1	H	71	GLN	CA-C-N	-6.17	113.73	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	71	GLN	C-N-CA	-6.17	113.73	123.24
1	E	78	GLY	N-CA-C	6.03	121.31	114.67
1	D	42	ASN	CA-C-N	-5.62	114.00	119.90
1	D	42	ASN	C-N-CA	-5.62	114.00	119.90
1	F	32	TYR	N-CA-C	5.43	120.31	113.25
1	A	42	ASN	CA-C-N	-5.38	114.38	119.76
1	A	42	ASN	C-N-CA	-5.38	114.38	119.76
1	F	110	ASP	N-CA-C	-5.37	105.43	111.28
1	G	131	ILE	CB-CA-C	-5.30	102.34	110.50
1	G	71	GLN	CA-C-N	-5.22	115.44	122.95
1	G	71	GLN	C-N-CA	-5.22	115.44	122.95
1	H	11	HIS	CA-C-N	-5.20	113.28	119.05
1	H	11	HIS	C-N-CA	-5.20	113.28	119.05
1	H	24	ILE	N-CA-C	5.11	115.67	108.36
1	A	2	GLN	N-CA-C	5.09	117.05	108.96

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	1095	0	1094	18	0
1	B	1095	0	1094	16	0
1	C	1095	0	1094	20	0
1	D	1095	0	1094	13	0
1	E	1095	0	1094	15	1
1	F	1095	0	1094	18	0
1	G	1095	0	1094	30	1
1	H	1095	0	1094	20	0
1	I	1095	0	1094	12	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
2	C	12	0	16	1	0
2	D	6	0	8	4	0
2	E	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	12	0	16	8	0
2	G	6	0	8	7	0
2	H	6	0	8	0	0
2	I	6	0	8	1	0
3	A	65	0	0	2	0
3	B	83	0	0	8	0
3	C	72	0	0	7	0
3	D	56	0	0	3	0
3	E	81	0	0	8	0
3	F	69	0	0	7	0
3	G	53	0	0	3	0
3	H	59	0	0	4	0
3	I	51	0	0	4	0
All	All	10510	0	9934	145	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 7.

All (145) 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:A:114:GLU:OE2	1:G:137:ARG:NH1	1.93	1.00
1:G:66:ARG:HH11	2:G:201:GOL:C3	1.75	0.99
1:H:137:ARG:O	3:H:530:HOH:O	1.80	0.99
2:G:201:GOL:O2	3:G:351:HOH:O	1.82	0.97
1:F:98:ARG:CB	2:F:202:GOL:H12	1.93	0.97
1:G:66:ARG:HH11	2:G:201:GOL:H31	1.29	0.95
1:F:72:HIS:HD2	3:F:333:HOH:O	1.46	0.95
1:G:66:ARG:NH1	2:G:201:GOL:H31	1.84	0.90
1:E:127:ARG:HH22	1:E:129:LYS:HE2	1.34	0.89
1:F:127:ARG:HH22	1:F:129:LYS:HE2	1.40	0.86
1:C:25:ARG:HB3	3:C:342:HOH:O	1.74	0.85
1:F:98:ARG:HB2	2:F:202:GOL:H12	1.59	0.84
1:I:71:GLN:O	3:I:339:HOH:O	1.93	0.84
2:E:201:GOL:H32	3:E:314:HOH:O	1.78	0.82
1:F:98:ARG:HB3	2:F:202:GOL:H12	1.62	0.82
1:I:127:ARG:HH22	1:I:129:LYS:HE2	1.45	0.80
1:A:127:ARG:HH22	1:A:129:LYS:HE2	1.47	0.79
1:D:29:GLU:O	2:D:201:GOL:H11	1.81	0.79
1:B:72:HIS:HD2	3:B:326:HOH:O	1.65	0.78
1:G:132:GLN:OE1	1:H:127:ARG:HD2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:GLN:NE2	3:F:367:HOH:O	2.16	0.77
1:B:98:ARG:HB3	3:B:312:HOH:O	1.85	0.76
1:B:98:ARG:CB	3:B:312:HOH:O	2.33	0.76
1:E:1:MET:N	3:E:351:HOH:O	2.16	0.76
1:G:66:ARG:NH1	2:G:201:GOL:C3	2.44	0.76
1:I:99:GLU:OE2	3:I:320:HOH:O	2.04	0.76
2:C:201:GOL:H11	3:C:368:HOH:O	1.86	0.75
1:D:127:ARG:HH22	1:D:129:LYS:HE2	1.48	0.75
1:E:98:ARG:HD2	1:I:15:PHE:CE2	2.23	0.73
1:B:71:GLN:NE2	3:B:371:HOH:O	2.22	0.72
1:H:72:HIS:HD2	3:H:547:HOH:O	1.73	0.71
2:A:201:GOL:H2	1:B:66:ARG:HH11	1.54	0.71
1:G:99:GLU:OE1	3:G:353:HOH:O	2.08	0.70
1:E:11:HIS:HD2	3:E:317:HOH:O	1.73	0.70
2:E:201:GOL:C3	3:E:314:HOH:O	2.37	0.70
1:I:72:HIS:HD2	3:I:333:HOH:O	1.75	0.69
1:A:78:GLY:O	1:G:25:ARG:NH1	2.25	0.68
1:F:98:ARG:HD3	3:F:366:HOH:O	1.94	0.67
1:D:127:ARG:NH2	1:D:129:LYS:HE2	2.10	0.66
1:I:11:HIS:HD2	3:I:314:HOH:O	1.79	0.65
1:A:11:HIS:HD2	3:A:308:HOH:O	1.78	0.65
1:D:1:MET:N	3:D:335:HOH:O	2.30	0.65
2:A:201:GOL:H2	1:B:66:ARG:NH1	2.11	0.64
1:G:127:ARG:HH22	1:G:129:LYS:HE2	1.61	0.64
1:H:1:MET:N	3:H:517:HOH:O	2.30	0.64
1:G:11:HIS:HD2	3:G:338:HOH:O	1.79	0.64
1:A:127:ARG:NH2	1:A:129:LYS:HE2	2.11	0.63
1:D:11:HIS:HE1	1:D:30:ASP:O	1.81	0.62
1:E:66:ARG:HH11	2:F:201:GOL:H2	1.65	0.62
1:H:127:ARG:NE	3:H:543:HOH:O	2.20	0.62
1:G:132:GLN:OE1	1:H:127:ARG:NH1	2.31	0.62
1:C:66:ARG:HH11	2:D:201:GOL:H2	1.64	0.61
1:G:11:HIS:HE1	1:G:30:ASP:O	1.85	0.60
1:G:127:ARG:NH2	1:G:129:LYS:HE2	2.16	0.59
1:C:127:ARG:HH22	1:C:129:LYS:HE2	1.67	0.59
1:A:135:SER:OG	1:B:105:HIS:HD2	1.86	0.59
1:B:11:HIS:HD2	3:B:315:HOH:O	1.84	0.59
1:C:135:SER:OG	1:D:105:HIS:HD2	1.87	0.58
1:E:105:HIS:HD2	1:F:135:SER:OG	1.86	0.58
1:A:30:ASP:OD1	1:A:72:HIS:HE1	1.86	0.57
1:E:11:HIS:HE1	1:E:30:ASP:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:HH22	1:B:129:LYS:HE2	1.70	0.57
1:E:66:ARG:NH1	2:F:201:GOL:H2	2.20	0.56
1:H:131:ILE:O	1:H:131:ILE:HG13	2.04	0.56
1:A:48:LEU:C	1:A:48:LEU:HD12	2.30	0.56
1:F:127:ARG:NH2	1:F:129:LYS:HE2	2.15	0.55
1:B:11:HIS:HE1	1:B:30:ASP:O	1.89	0.55
1:G:130:ASP:OD1	1:G:130:ASP:N	2.39	0.55
1:A:20:ARG:O	1:H:129:LYS:HB2	2.07	0.54
1:C:86:ARG:HD3	3:C:340:HOH:O	2.07	0.54
1:E:72:HIS:HD2	3:E:337:HOH:O	1.91	0.54
1:I:11:HIS:HE1	1:I:30:ASP:O	1.92	0.53
1:A:72:HIS:HD2	3:A:362:HOH:O	1.90	0.53
1:B:98:ARG:HB2	3:B:312:HOH:O	2.05	0.53
1:B:116:GLN:HB3	1:B:120:ARG:NH1	2.23	0.52
1:G:48:LEU:C	1:G:48:LEU:HD12	2.34	0.52
1:E:66:ARG:HH11	2:F:201:GOL:C2	2.23	0.52
1:G:66:ARG:NH1	2:G:201:GOL:H32	2.24	0.52
1:A:105:HIS:HD2	1:B:135:SER:OG	1.93	0.51
1:C:40:GLN:HE22	1:G:40:GLN:HE22	1.57	0.51
1:E:71:GLN:NE2	3:E:380:HOH:O	2.35	0.51
1:C:66:ARG:NH1	2:D:201:GOL:H2	2.26	0.51
1:A:71:GLN:NE2	3:B:383:HOH:O	2.44	0.51
1:C:105:HIS:HE1	3:C:352:HOH:O	1.92	0.51
1:C:66:ARG:HH11	2:D:201:GOL:C2	2.25	0.50
1:G:135:SER:OG	1:H:105:HIS:HD2	1.94	0.50
1:C:105:HIS:HD2	1:D:135:SER:OG	1.94	0.50
1:G:66:ARG:HH11	2:G:201:GOL:H32	1.65	0.50
1:D:99:GLU:OE2	3:D:321:HOH:O	2.20	0.49
1:F:11:HIS:HD2	3:F:306:HOH:O	1.95	0.49
1:C:30:ASP:OD1	1:C:72:HIS:HE1	1.96	0.49
1:H:11:HIS:HE1	1:H:30:ASP:O	1.95	0.49
1:H:30:ASP:OD1	1:H:72:HIS:HE1	1.95	0.49
1:E:135:SER:OG	1:F:105:HIS:HD2	1.96	0.48
1:F:11:HIS:HE1	1:F:30:ASP:O	1.96	0.48
1:H:29:GLU:H	1:H:29:GLU:CD	2.21	0.48
1:C:86:ARG:CD	3:C:340:HOH:O	2.61	0.48
1:H:48:LEU:HD12	1:H:48:LEU:C	2.39	0.48
1:I:130:ASP:OD1	1:I:130:ASP:N	2.46	0.48
1:G:42:ASN:HB3	1:G:45:LEU:HD12	1.96	0.47
1:G:131:ILE:O	1:G:131:ILE:HG13	2.12	0.47
1:E:127:ARG:NH2	1:E:129:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:ARG:HB2	2:F:202:GOL:C1	2.39	0.46
1:B:30:ASP:OD1	1:B:72:HIS:HE1	1.98	0.46
1:H:127:ARG:HH22	1:H:129:LYS:HE2	1.80	0.46
1:A:11:HIS:HE1	1:A:30:ASP:O	1.98	0.46
1:I:38:TYR:CD1	2:I:201:GOL:H32	2.51	0.46
1:E:132:GLN:OE1	1:F:127:ARG:NH1	2.41	0.45
1:D:49:VAL:HG12	1:D:56:ILE:HD11	1.96	0.45
1:I:127:ARG:NH2	1:I:129:LYS:HE2	2.23	0.45
1:I:11:HIS:HB3	1:I:12:PRO:HD3	1.99	0.45
1:B:99:GLU:OE1	3:B:377:HOH:O	2.21	0.45
1:A:21:THR:HB	1:A:24:ILE:HD12	1.97	0.45
1:C:15:PHE:CD2	1:H:98:ARG:HD2	2.53	0.44
1:E:105:HIS:HE1	3:E:322:HOH:O	2.01	0.44
1:D:48:LEU:HD12	1:D:48:LEU:C	2.43	0.43
1:G:131:ILE:HG22	1:H:109:LEU:HD23	2.00	0.43
1:G:30:ASP:OD1	1:G:72:HIS:HE1	2.01	0.43
1:I:30:ASP:OD1	1:I:72:HIS:HE1	2.01	0.43
1:C:132:GLN:OE1	1:D:127:ARG:NH1	2.45	0.43
1:G:105:HIS:HD2	1:H:135:SER:OG	2.02	0.43
1:A:1:MET:HE2	1:A:1:MET:HB2	1.95	0.42
1:G:29:GLU:HA	1:G:34:PHE:CG	2.54	0.42
1:C:48:LEU:C	1:C:48:LEU:HD12	2.44	0.42
1:F:105:HIS:HE1	3:F:340:HOH:O	2.02	0.42
2:F:201:GOL:C1	3:F:362:HOH:O	2.67	0.42
1:G:112:ALA:O	1:G:116:GLN:HG2	2.20	0.42
1:G:127:ARG:HD2	1:H:132:GLN:OE1	2.19	0.42
1:B:42:ASN:ND2	1:B:63:HIS:H	2.17	0.42
1:C:11:HIS:HE1	1:C:30:ASP:O	2.03	0.42
1:D:72:HIS:HD2	3:D:323:HOH:O	2.02	0.41
1:F:11:HIS:HB3	1:F:12:PRO:HD3	2.03	0.41
1:D:11:HIS:HB2	1:D:35:PHE:CE2	2.56	0.41
1:C:40:GLN:NE2	1:G:40:GLN:HE22	2.17	0.41
1:G:109:LEU:HD23	1:G:109:LEU:HA	1.86	0.41
1:C:72:HIS:HD2	3:C:363:HOH:O	2.03	0.41
1:C:120:ARG:HH12	1:F:22:PRO:HB3	1.85	0.41
1:F:72:HIS:CD2	3:F:333:HOH:O	2.37	0.41
1:A:11:HIS:HB3	1:A:12:PRO:HD3	2.03	0.41
1:H:1:MET:HE2	1:H:1:MET:HB2	1.96	0.41
1:G:3:LEU:CD1	1:G:88:MET:HG2	2.51	0.40
1:A:32:TYR:HB3	1:A:33:PRO:HD3	2.03	0.40
1:A:20:ARG:HB2	1:H:129:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:HIS:CD2	3:C:363:HOH:O	2.75	0.40
2:E:201:GOL:H31	3:E:314:HOH:O	2.15	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)
1:E:79:TYR:OH	1:G:90:ASP:OD2[8_675]	1.76	0.44

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	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
1	B	135/141 (96%)	134 (99%)	1 (1%)	0	100	100
1	C	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
1	D	135/141 (96%)	132 (98%)	3 (2%)	0	100	100
1	E	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
1	F	135/141 (96%)	134 (99%)	1 (1%)	0	100	100
1	G	135/141 (96%)	132 (98%)	3 (2%)	0	100	100
1	H	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
1	I	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
All	All	1215/1269 (96%)	1197 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	109/111 (98%)	108 (99%)	1 (1%)	70	82
1	B	109/111 (98%)	108 (99%)	1 (1%)	70	82
1	C	109/111 (98%)	108 (99%)	1 (1%)	70	82
1	D	109/111 (98%)	108 (99%)	1 (1%)	70	82
1	E	109/111 (98%)	109 (100%)	0	100	100
1	F	109/111 (98%)	108 (99%)	1 (1%)	70	82
1	G	109/111 (98%)	107 (98%)	2 (2%)	51	66
1	H	109/111 (98%)	107 (98%)	2 (2%)	51	66
1	I	109/111 (98%)	107 (98%)	2 (2%)	51	66
All	All	981/999 (98%)	970 (99%)	11 (1%)	65	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	76	ASP
1	C	76	ASP
1	D	76	ASP
1	F	98	ARG
1	G	29	GLU
1	G	110	ASP
1	H	29	GLU
1	H	76	ASP
1	I	76	ASP
1	I	130	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	11	HIS

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Mol	Chain	Res	Type
1	A	42	ASN
1	A	72	HIS
1	A	105	HIS
1	B	2	GLN
1	B	11	HIS
1	B	42	ASN
1	B	72	HIS
1	B	105	HIS
1	C	2	GLN
1	C	11	HIS
1	C	40	GLN
1	C	42	ASN
1	C	72	HIS
1	C	105	HIS
1	D	2	GLN
1	D	11	HIS
1	D	42	ASN
1	D	72	HIS
1	D	105	HIS
1	E	2	GLN
1	E	11	HIS
1	E	42	ASN
1	E	72	HIS
1	E	105	HIS
1	F	2	GLN
1	F	11	HIS
1	F	40	GLN
1	F	42	ASN
1	F	72	HIS
1	F	105	HIS
1	G	2	GLN
1	G	11	HIS
1	G	42	ASN
1	G	72	HIS
1	G	105	HIS
1	H	2	GLN
1	H	11	HIS
1	H	42	ASN
1	H	72	HIS
1	H	105	HIS
1	I	2	GLN
1	I	11	HIS

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Mol	Chain	Res	Type
1	I	42	ASN
1	I	72	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	GOL	B	201	-	5,5,5	0.73	0	5,5,5	1.79	2 (40%)
2	GOL	D	201	-	5,5,5	0.62	0	5,5,5	0.88	0
2	GOL	G	201	-	5,5,5	0.62	0	5,5,5	1.89	2 (40%)
2	GOL	I	201	-	5,5,5	0.68	0	5,5,5	1.16	1 (20%)
2	GOL	C	201	-	5,5,5	0.47	0	5,5,5	1.34	1 (20%)
2	GOL	E	201	-	5,5,5	0.83	0	5,5,5	1.22	1 (20%)
2	GOL	F	202	-	5,5,5	0.79	0	5,5,5	1.72	1 (20%)
2	GOL	C	202	-	5,5,5	0.38	0	5,5,5	0.84	0
2	GOL	H	201	-	5,5,5	0.50	0	5,5,5	0.79	0
2	GOL	A	201	-	5,5,5	1.11	0	5,5,5	0.99	1 (20%)
2	GOL	F	201	-	5,5,5	0.26	0	5,5,5	0.61	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
2	GOL	B	201	-	-	0/4/4/4	-
2	GOL	D	201	-	-	2/4/4/4	-
2	GOL	G	201	-	-	2/4/4/4	-
2	GOL	I	201	-	-	2/4/4/4	-
2	GOL	C	201	-	-	0/4/4/4	-
2	GOL	E	201	-	-	2/4/4/4	-
2	GOL	F	202	-	-	2/4/4/4	-
2	GOL	C	202	-	-	2/4/4/4	-
2	GOL	H	201	-	-	4/4/4/4	-
2	GOL	A	201	-	-	2/4/4/4	-
2	GOL	F	201	-	-	2/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	GOL	C3-C2-C1	-3.14	100.29	111.80
2	F	202	GOL	O1-C1-C2	-3.04	96.69	110.38
2	B	201	GOL	O1-C1-C2	-2.53	98.99	110.38
2	B	201	GOL	C3-C2-C1	-2.49	102.66	111.80
2	C	201	GOL	C3-C2-C1	-2.31	103.32	111.80
2	E	201	GOL	O2-C2-C1	2.28	118.63	109.18
2	G	201	GOL	O2-C2-C1	2.15	118.07	109.18
2	A	201	GOL	O2-C2-C1	2.09	117.85	109.18
2	I	201	GOL	O2-C2-C1	2.03	117.60	109.18

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	202	GOL	C1-C2-C3-O3
2	D	201	GOL	C1-C2-C3-O3
2	E	201	GOL	C1-C2-C3-O3
2	F	202	GOL	O1-C1-C2-C3
2	G	201	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	H	201	GOL	O1-C1-C2-O2
2	H	201	GOL	O1-C1-C2-C3
2	H	201	GOL	C1-C2-C3-O3
2	A	201	GOL	O1-C1-C2-O2
2	D	201	GOL	O2-C2-C3-O3
2	F	201	GOL	O2-C2-C3-O3
2	A	201	GOL	O1-C1-C2-C3
2	F	201	GOL	C1-C2-C3-O3
2	I	201	GOL	O1-C1-C2-C3
2	C	202	GOL	O2-C2-C3-O3
2	F	202	GOL	O1-C1-C2-O2
2	G	201	GOL	O2-C2-C3-O3
2	H	201	GOL	O2-C2-C3-O3
2	I	201	GOL	O1-C1-C2-O2
2	E	201	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	GOL	4	0
2	G	201	GOL	7	0
2	I	201	GOL	1	0
2	C	201	GOL	1	0
2	E	201	GOL	3	0
2	F	202	GOL	4	0
2	A	201	GOL	2	0
2	F	201	GOL	4	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, 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	137/141 (97%)	-0.13	2 (1%) 72 70	27, 40, 65, 73	0
1	B	137/141 (97%)	-0.18	1 (0%) 84 83	25, 37, 64, 82	0
1	C	137/141 (97%)	0.05	4 (2%) 53 51	27, 43, 74, 94	0
1	D	137/141 (97%)	-0.02	2 (1%) 72 70	28, 45, 71, 86	0
1	E	137/141 (97%)	-0.15	2 (1%) 72 70	27, 38, 67, 84	0
1	F	137/141 (97%)	-0.01	4 (2%) 53 51	29, 44, 72, 85	0
1	G	137/141 (97%)	0.20	10 (7%) 21 18	27, 44, 75, 92	0
1	H	137/141 (97%)	0.23	11 (8%) 18 16	25, 45, 79, 99	0
1	I	137/141 (97%)	0.09	3 (2%) 62 60	31, 48, 77, 89	0
All	All	1233/1269 (97%)	0.01	39 (3%) 50 47	25, 43, 73, 99	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLU	5.7
1	G	111	ALA	3.4
1	G	27	ARG	3.3
1	C	112	ALA	3.2
1	D	129	LYS	3.1
1	F	23	GLY	3.1
1	H	127	ARG	3.1
1	H	131	ILE	3.0
1	H	129	LYS	3.0
1	I	129	LYS	3.0
1	H	103	LYS	3.0
1	I	76	ASP	2.9
1	H	113	GLU	2.9
1	G	137	ARG	2.8
1	C	111	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	23	GLY	2.7
1	D	27	ARG	2.6
1	G	110	ASP	2.6
1	G	132	GLN	2.5
1	C	129	LYS	2.5
1	H	132	GLN	2.5
1	E	1	MET	2.4
1	E	113	GLU	2.4
1	I	81	GLY	2.4
1	H	120	ARG	2.4
1	G	129	LYS	2.3
1	B	129	LYS	2.3
1	F	113	GLU	2.3
1	F	1	MET	2.2
1	G	113	GLU	2.2
1	H	27	ARG	2.2
1	A	22	PRO	2.2
1	H	116	GLN	2.2
1	G	1	MET	2.1
1	H	23	GLY	2.1
1	H	128	ARG	2.1
1	F	129	LYS	2.0
1	A	1	MET	2.0
1	G	131	ILE	2.0

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 oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	H	201	6/6	0.75	0.31	51,55,59,63	6
2	GOL	E	201	6/6	0.79	0.19	31,36,44,45	6
2	GOL	C	202	6/6	0.82	0.29	50,54,59,62	6
2	GOL	F	202	6/6	0.84	0.28	38,39,43,50	0
2	GOL	G	201	6/6	0.86	0.19	31,39,43,47	6
2	GOL	I	201	6/6	0.87	0.19	36,43,45,47	6
2	GOL	B	201	6/6	0.88	0.16	29,31,33,39	6
2	GOL	C	201	6/6	0.89	0.15	29,33,35,41	6
2	GOL	A	201	6/6	0.90	0.14	45,48,53,55	0
2	GOL	F	201	6/6	0.91	0.13	36,42,42,49	6
2	GOL	D	201	6/6	0.92	0.12	37,41,44,44	6

6.5 Other polymers [i](#)

There are no such residues in this entry.