



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 09:13 PM EDT

PDB ID : 3R5D  
Title : Pseudomonas aeruginosa DapD (PA3666) apoprotein  
Authors : Sandalova, T.; Schnell, R.; Schneider, G.  
Deposited on : 2011-03-18  
Resolution : 1.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

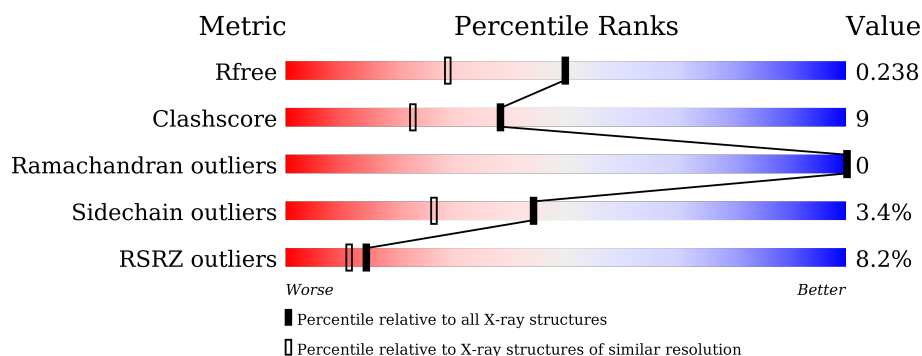
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	347	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	B	347	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
1	C	347	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 8%</div> </div> </div>
1	D	347	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	E	347	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	F	347	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 8%</div> </div> </div>

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	A	345	-	-	-	X
2	GOL	E	345	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14905 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 Tetrahydrodipicolinate N-succinyletransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	2	0
			2366	1507	405	447	7			
1	B	320	Total	C	N	O	S	0	2	0
			2366	1507	405	447	7			
1	C	319	Total	C	N	O	S	0	1	0
			2358	1502	404	445	7			
1	D	320	Total	C	N	O	S	0	2	0
			2370	1509	408	446	7			
1	E	320	Total	C	N	O	S	0	2	0
			2366	1507	405	447	7			
1	F	320	Total	C	N	O	S	0	1	0
			2362	1504	405	446	7			

There are 18 discrepancies between the modelled and reference sequences:

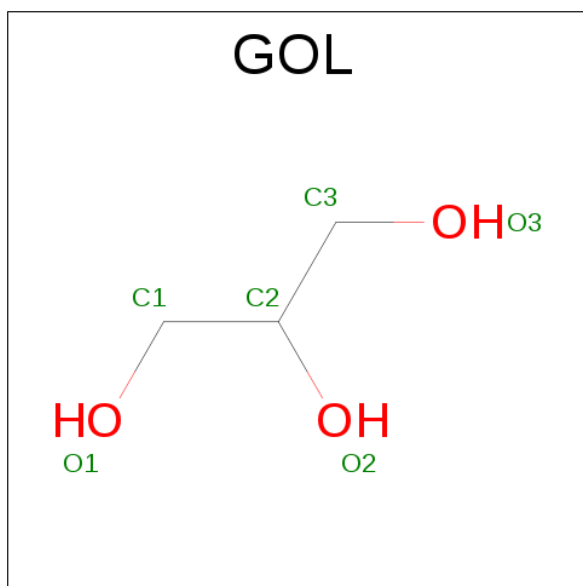
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
A	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
A	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
B	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
B	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
C	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
C	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
C	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
D	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
D	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
D	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
E	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
E	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
E	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
F	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
F	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

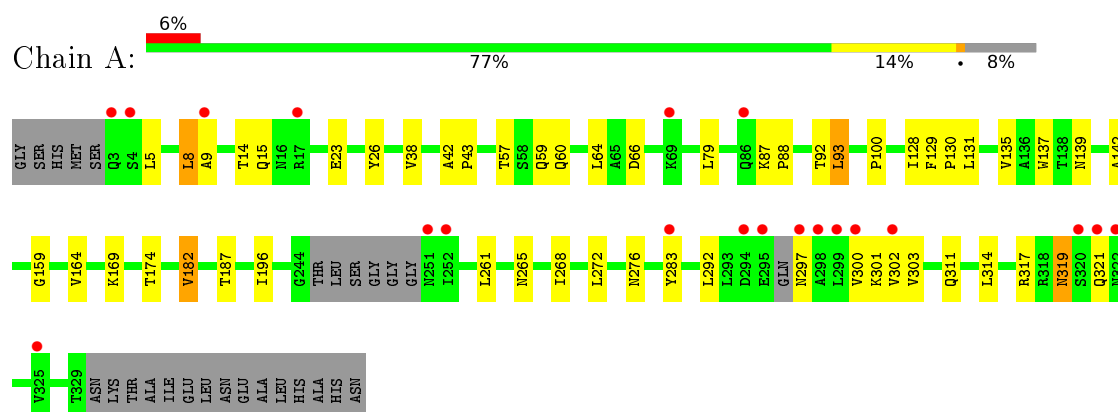
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	143	Total	O	0	0
			143	143		
3	C	89	Total	O	0	0
			89	89		
3	D	120	Total	O	0	0
			120	120		
3	E	147	Total	O	0	0
			147	147		
3	F	94	Total	O	0	0
			94	94		

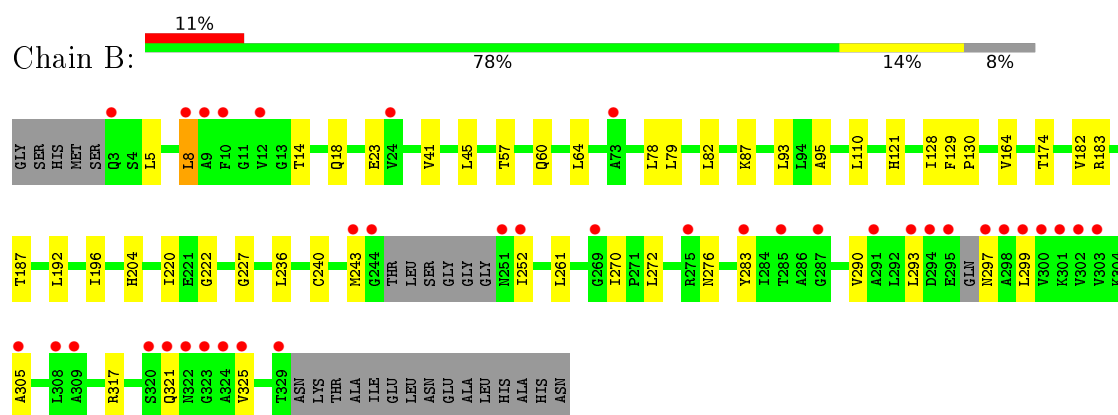
### 3 Residue-property plots [i](#)

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

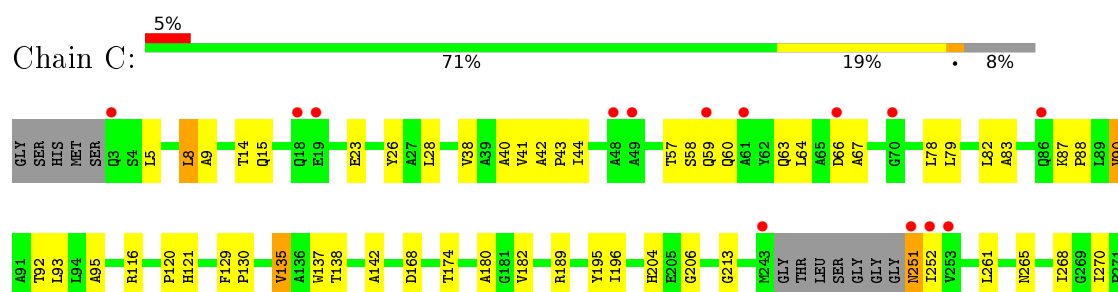
- Molecule 1: Tetrahydrodipicolinate N-succinyletransferase

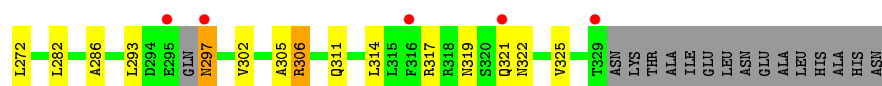


- Molecule 1: Tetrahydrodipicolinate N-succinyletransferase

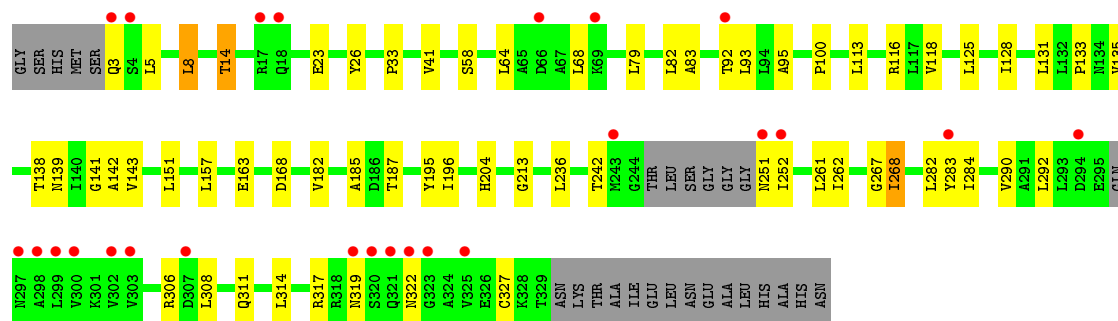
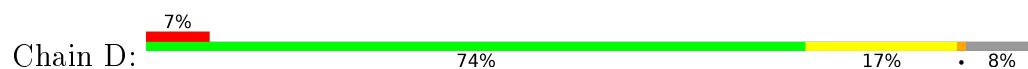


- Molecule 1: Tetrahydrodipicolinate N-succinyletransferase

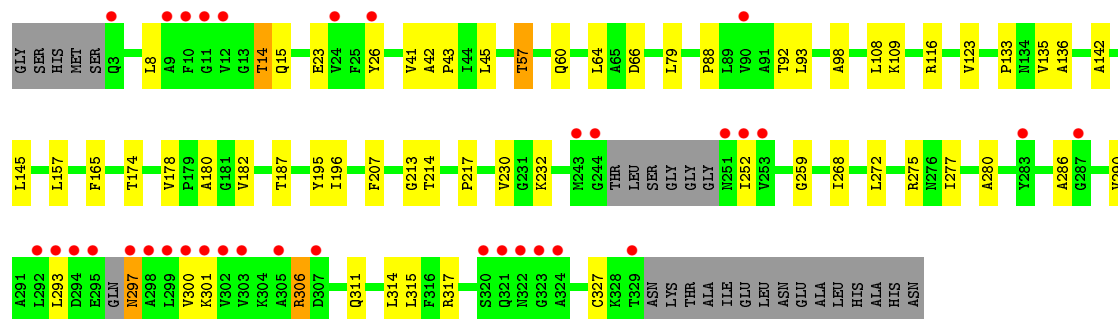
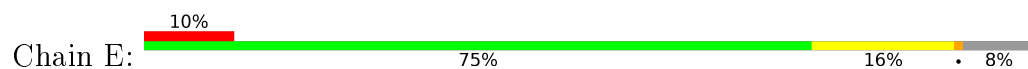




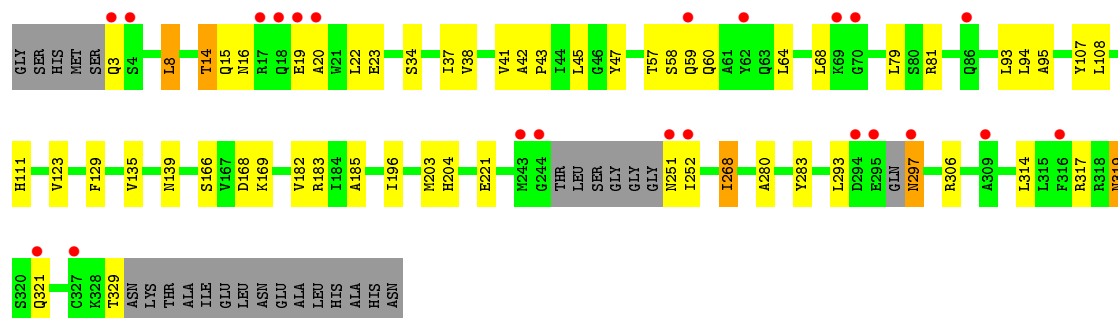
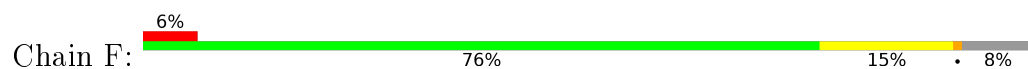
• Molecule 1: Tetrahydrodipicolinate N-succinyletransferase



• Molecule 1: Tetrahydrodipicolinate N-succinyletransferase



• Molecule 1: Tetrahydrodipicolinate N-succinyletransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.04Å 102.00Å 134.90Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	24.38 – 1.80 24.38 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (24.38-1.80) 94.9 (24.38-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.202 , 0.236 0.209 , 0.238	Depositor DCC
$R_{free}$ test set	9990 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 31.7	EDS
Estimated twinning fraction	0.507 for H, K, L 0.493 for H, -K, -L 0.277 for h,-k,-l	Xtriage
Reported twinning fraction	0.507 for H, K, L 0.493 for H, -K, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 197589 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14905	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/2408	0.56	0/3268
1	B	0.38	0/2408	0.55	0/3268
1	C	0.38	0/2397	0.56	0/3253
1	D	0.38	0/2412	0.58	1/3272 (0.0%)
1	E	0.38	0/2408	0.56	0/3268
1	F	0.38	0/2401	0.58	0/3258
All	All	0.38	0/14434	0.56	1/19587 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	ARG	NE-CZ-NH2	-6.36	117.12	120.30

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	2366	0	2422	45	0
1	B	2366	0	2422	39	0
1	C	2358	0	2412	59	0
1	D	2370	0	2428	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2366	0	2422	48	0
1	F	2362	0	2415	44	0
2	A	6	0	8	2	0
2	E	6	0	8	4	0
3	A	112	0	0	0	0
3	B	143	0	0	1	0
3	C	89	0	0	3	0
3	D	120	0	0	2	0
3	E	147	0	0	1	0
3	F	94	0	0	0	0
All	All	14905	0	14537	262	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 9.

All (262) 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:14:THR:HG22	1:A:87:LYS:NZ	1.73	1.01
1:B:14:THR:HG22	1:B:87:LYS:HZ1	1.31	0.95
1:A:139:ASN:HB2	2:A:345:GOL:H12	1.54	0.88
1:A:14:THR:HG22	1:A:87:LYS:HZ1	1.38	0.87
1:C:8:LEU:HD13	1:C:93:LEU:HD22	1.58	0.86
1:C:26:TYR:OH	1:C:92:THR:HG21	1.74	0.86
1:B:14:THR:HG22	1:B:87:LYS:NZ	1.91	0.85
1:F:57:THR:HG22	1:F:59:GLN:H	1.43	0.83
1:C:8:LEU:HD13	1:C:93:LEU:CD2	2.09	0.82
1:F:45:LEU:HD21	1:F:64:LEU:HD11	1.62	0.82
1:B:14:THR:HG23	1:B:23:GLU:OE1	1.82	0.80
1:E:174:THR:HG22	1:E:178:VAL:HG22	1.66	0.76
1:B:174[A]:THR:HG21	1:B:187:THR:HG21	1.68	0.76
1:C:14:THR:HG23	1:C:23:GLU:OE1	1.87	0.74
1:A:57:THR:HG22	1:A:60:GLN:HE21	1.52	0.74
1:E:41:VAL:HG13	1:E:64:LEU:CD2	2.18	0.73
1:A:14:THR:HG22	1:A:87:LYS:HZ3	1.52	0.73
1:D:100:PRO:O	1:D:131:LEU:HD11	1.89	0.72
1:B:5:LEU:HD22	1:B:95:ALA:HA	1.72	0.71
1:C:41:VAL:HG13	1:C:64:LEU:HD22	1.72	0.70
1:F:38:VAL:O	1:F:42:ALA:HB2	1.91	0.70
1:F:3:GLN:OE1	1:F:95:ALA:HB1	1.93	0.69
1:F:182:VAL:HG11	1:F:196:ILE:HG21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HD12	1:C:9:ALA:N	2.09	0.68
1:A:164:VAL:O	1:C:174[B]:THR:HG21	1.94	0.68
1:C:78:LEU:O	1:C:82:LEU:HD13	1.94	0.68
1:A:174[B]:THR:HG21	1:B:164:VAL:O	1.95	0.66
1:B:272:LEU:HD22	1:B:276:ASN:HD22	1.61	0.66
1:C:42:ALA:HB3	1:C:43:PRO:HD3	1.77	0.65
1:C:14:THR:HG22	1:C:87:LYS:NZ	2.10	0.65
1:D:135:VAL:HG11	1:D:142:ALA:HB1	1.79	0.64
1:F:319:ASN:HD22	1:F:321:GLN:H	1.45	0.64
1:E:41:VAL:HG13	1:E:64:LEU:HD22	1.78	0.64
1:E:92[A]:THR:OG1	1:E:108:LEU:HD22	1.98	0.64
1:F:14:THR:HG23	1:F:23:GLU:OE1	1.97	0.64
1:E:280:ALA:HB1	1:F:283:TYR:CE1	2.33	0.64
1:E:57[B]:THR:H	1:E:60:GLN:HE21	1.46	0.63
1:E:57[A]:THR:H	1:E:60:GLN:HE21	1.46	0.63
1:A:26:TYR:OH	1:A:92[B]:THR:HG21	1.98	0.63
1:F:34:SER:O	1:F:38:VAL:HG23	1.98	0.62
1:C:14:THR:OG1	1:C:23:GLU:HG3	2.01	0.60
1:D:267:GLY:HA3	1:D:283:TYR:CD1	2.36	0.60
1:E:41:VAL:HG12	1:E:45:LEU:HD12	1.84	0.60
1:F:8:LEU:HB2	1:F:93:LEU:CD2	2.32	0.59
1:D:8:LEU:C	1:D:8:LEU:HD12	2.22	0.59
1:A:139:ASN:CB	2:A:345:GOL:H12	2.30	0.59
1:C:15:GLN:HE21	1:C:88:PRO:HG3	1.67	0.59
1:E:41:VAL:HG13	1:E:64:LEU:HD21	1.84	0.59
1:C:251:ASN:HD22	1:C:251:ASN:N	2.00	0.59
1:C:57:THR:HG22	1:C:60:GLN:HG3	1.85	0.59
1:A:174[B]:THR:CG2	1:B:164:VAL:O	2.51	0.58
1:B:182:VAL:HG22	1:B:196:ILE:HG22	1.84	0.58
1:A:265:ASN:ND2	1:B:283:TYR:OH	2.30	0.58
1:D:267:GLY:HA3	1:D:283:TYR:CE1	2.39	0.58
1:E:98:ALA:O	1:E:109:LYS:NZ	2.36	0.58
1:E:41:VAL:HG12	1:E:45:LEU:CD1	2.34	0.58
1:C:14:THR:HG22	1:C:87:LYS:HZ3	1.65	0.58
1:B:41:VAL:HG22	1:B:64:LEU:HD22	1.85	0.58
1:A:14:THR:HG23	1:A:23:GLU:OE1	2.04	0.57
1:D:5:LEU:HD22	1:D:95:ALA:HA	1.85	0.57
1:B:174[A]:THR:HG21	1:B:187:THR:CG2	2.34	0.57
1:E:116:ARG:NH2	1:E:180:ALA:O	2.34	0.56
1:D:290:VAL:HG11	1:D:327:CYS:HB2	1.88	0.56
1:C:41:VAL:HG13	1:C:64:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:VAL:HG11	1:E:196:ILE:HG21	1.87	0.56
1:C:129:PHE:HB2	1:C:130:PRO:HD3	1.87	0.56
1:D:182:VAL:HG11	1:D:196:ILE:HG21	1.88	0.56
1:D:252:ILE:O	1:D:252:ILE:HD12	2.05	0.56
1:F:252:ILE:O	1:F:252:ILE:HD12	2.06	0.56
1:C:14:THR:HG21	3:C:437:HOH:O	2.06	0.56
1:C:137:TRP:CZ3	1:C:142:ALA:HB2	2.41	0.55
1:E:187:THR:HG23	1:F:166:SER:HA	1.89	0.55
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.89	0.55
1:A:164:VAL:O	1:C:174[B]:THR:CG2	2.55	0.55
1:F:8:LEU:HB2	1:F:93:LEU:HD22	1.88	0.55
1:A:311:GLN:HB2	1:A:314:LEU:HD11	1.90	0.54
1:B:290:VAL:HG22	1:B:325:VAL:HG12	1.88	0.54
1:D:133:PRO:O	1:D:135:VAL:HG23	2.06	0.54
1:D:100:PRO:HB2	1:D:131:LEU:CD1	2.38	0.54
1:B:129:PHE:HB2	1:B:130:PRO:HD3	1.89	0.54
1:C:40:ALA:HB1	1:C:67:ALA:HB1	1.89	0.54
1:F:182:VAL:HG11	1:F:196:ILE:CG2	2.38	0.54
1:A:57:THR:H	1:A:60:GLN:HE21	1.54	0.54
1:A:8:LEU:HB2	1:A:93:LEU:HD22	1.90	0.54
1:B:57:THR:H	1:B:60:GLN:HE21	1.55	0.54
1:C:182:VAL:HG22	1:C:196:ILE:HG22	1.89	0.54
1:E:57[B]:THR:H	1:E:60:GLN:NE2	2.06	0.54
1:D:41:VAL:HG22	1:D:64:LEU:HD22	1.90	0.53
1:E:14:THR:HG23	1:E:23:GLU:HG3	1.89	0.53
1:E:57[A]:THR:H	1:E:60:GLN:NE2	2.06	0.53
1:D:113:LEU:HD23	1:D:118:VAL:HG23	1.91	0.53
1:F:57:THR:CG2	1:F:58:SER:N	2.71	0.53
1:D:82:LEU:HD12	1:E:157:LEU:HD21	1.90	0.53
1:F:68:LEU:HD12	1:F:79:LEU:CD1	2.39	0.53
1:E:290:VAL:HG11	1:E:327:CYS:HB2	1.90	0.53
1:F:47:TYR:CG	1:F:93:LEU:HD12	2.44	0.53
1:B:8:LEU:HB2	1:B:93:LEU:HD22	1.90	0.53
1:D:14:THR:HG21	3:D:382:HOH:O	2.09	0.52
1:A:129:PHE:O	1:A:169:LYS:NZ	2.23	0.52
1:C:319:ASN:HD22	1:C:322:ASN:H	1.56	0.52
1:E:314:LEU:HD22	1:E:327:CYS:SG	2.48	0.52
1:A:292:LEU:O	1:A:300:VAL:HG12	2.10	0.52
1:E:133:PRO:O	1:E:135:VAL:HG23	2.10	0.52
1:B:321:GLN:HE21	1:C:302:VAL:HG11	1.74	0.52
1:E:26:TYR:OH	1:E:92[A]:THR:HG21	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ARG:HD3	1:C:206:GLY:O	2.10	0.52
1:C:57:THR:HG23	1:C:59:GLN:N	2.24	0.51
1:D:292:LEU:HD13	1:D:308:LEU:HD21	1.92	0.51
1:E:286:ALA:HB1	1:E:306:ARG:HB3	1.92	0.51
1:B:290:VAL:HG22	1:B:325:VAL:CG1	2.40	0.51
1:C:268:ILE:HG21	1:C:272:LEU:HD11	1.93	0.51
1:F:185:ALA:HB1	1:F:204:HIS:CE1	2.46	0.51
1:A:100:PRO:O	1:A:131:LEU:HD11	2.11	0.50
1:A:265:ASN:HD22	1:B:283:TYR:HH	1.52	0.50
1:D:185:ALA:HB1	1:D:204:HIS:CE1	2.47	0.50
1:C:116:ARG:HD3	3:C:376:HOH:O	2.11	0.50
1:E:136:ALA:HB2	1:E:145:LEU:HD23	1.91	0.50
1:F:94:LEU:HD11	1:F:108:LEU:HD23	1.92	0.50
1:A:57:THR:HG23	1:A:60:GLN:H	1.77	0.50
1:C:28:LEU:HD11	3:C:480:HOH:O	2.12	0.50
1:D:26:TYR:OH	1:D:92[A]:THR:HG21	2.12	0.50
1:C:189:ARG:HD2	1:C:204:HIS:O	2.12	0.50
1:D:187:THR:OG1	1:E:165:PHE:HA	2.12	0.50
1:C:116:ARG:NH2	1:C:180:ALA:O	2.43	0.50
1:D:139:ASN:HB2	2:E:345:GOL:H31	1.94	0.50
1:D:282:LEU:HD11	1:D:284:ILE:HG23	1.93	0.49
1:C:90:VAL:HG13	1:C:92:THR:HG23	1.94	0.49
1:F:268:ILE:HG13	1:F:268:ILE:O	2.11	0.49
1:C:5:LEU:HD12	1:C:38:VAL:CG2	2.42	0.49
1:B:78:LEU:O	1:B:82:LEU:HD13	2.13	0.49
1:D:143:VAL:HG11	1:D:151:LEU:HD12	1.94	0.49
1:D:8:LEU:HB2	1:D:93:LEU:HD22	1.94	0.49
1:D:261:LEU:HD13	1:D:261:LEU:O	2.13	0.49
1:F:41:VAL:HG22	1:F:64:LEU:HD22	1.94	0.49
1:E:41:VAL:CG1	1:E:45:LEU:CD1	2.91	0.49
1:F:8:LEU:HD21	1:F:37:ILE:CG2	2.42	0.49
1:C:5:LEU:HD23	1:C:95:ALA:HA	1.94	0.49
1:D:283:TYR:CE1	1:F:280:ALA:HB1	2.47	0.49
1:C:44:ILE:HD13	1:C:63:GLN:HB3	1.95	0.48
1:B:8:LEU:C	1:B:8:LEU:HD12	2.33	0.48
1:A:159:GLY:HA2	1:C:87:LYS:HZ2	1.79	0.48
1:A:8:LEU:HD12	1:A:9:ALA:N	2.28	0.48
1:C:135:VAL:HG12	1:C:137:TRP:CE2	2.48	0.48
1:C:120:PRO:O	1:C:121:HIS:HB2	2.14	0.48
1:E:217:PRO:HD2	1:E:232:LYS:HG3	1.96	0.48
1:E:293:LEU:HD13	1:E:297:ASN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:C	1:C:93:LEU:HD23	2.35	0.47
1:F:57:THR:H	1:F:60:GLN:HE21	1.62	0.47
1:B:204:HIS:H	1:B:204:HIS:CD2	2.31	0.47
1:A:265:ASN:HB2	1:B:283:TYR:OH	2.15	0.47
1:F:57:THR:HG22	1:F:58:SER:N	2.29	0.47
1:D:319:ASN:HD22	1:D:322:ASN:H	1.61	0.47
1:B:110:LEU:HB3	1:B:192:LEU:HG	1.96	0.47
1:A:319:ASN:HD22	1:A:321:GLN:H	1.61	0.47
1:C:93:LEU:HD23	1:C:93:LEU:N	2.30	0.47
1:F:16:ASN:ND2	1:F:20:ALA:HB3	2.30	0.47
1:D:311:GLN:HB2	1:D:314:LEU:HD11	1.96	0.47
1:D:125:LEU:HD22	1:D:128:ILE:HD12	1.96	0.47
1:C:251:ASN:ND2	1:C:251:ASN:N	2.62	0.46
1:C:252:ILE:HD12	1:C:252:ILE:O	2.15	0.46
1:A:128:ILE:HG23	1:A:129:PHE:HD1	1.80	0.46
1:A:137:TRP:CZ3	1:A:142:ALA:HB2	2.49	0.46
1:C:195:TYR:O	1:C:213:GLY:HA3	2.15	0.46
1:C:293:LEU:HD13	1:C:297:ASN:HB2	1.96	0.46
1:D:282:LEU:HD12	1:D:283:TYR:N	2.30	0.46
1:E:214:THR:HG22	1:E:230:VAL:HB	1.96	0.46
1:E:64:LEU:HB3	1:E:79:LEU:HD13	1.98	0.46
1:A:283:TYR:OH	1:C:265:ASN:ND2	2.46	0.46
1:F:42:ALA:HB3	1:F:43:PRO:HD3	1.98	0.46
1:D:68:LEU:HD12	1:D:79:LEU:CD1	2.46	0.45
1:F:22:LEU:HD22	1:F:135:VAL:HG22	1.97	0.45
1:B:174[A]:THR:HG21	1:B:187:THR:CB	2.46	0.45
1:B:183:ARG:HD2	1:C:168:ASP:OD1	2.17	0.45
1:C:64:LEU:HB3	1:C:79:LEU:HD13	1.97	0.45
1:E:311:GLN:HB2	1:E:314:LEU:HD11	1.98	0.45
2:E:345:GOL:H12	1:F:139:ASN:HB3	1.98	0.45
1:A:64:LEU:HB3	1:A:79:LEU:HD13	1.97	0.45
1:F:293:LEU:HD13	1:F:297:ASN:HB2	1.98	0.45
1:A:272:LEU:HD22	1:A:276:ASN:HD22	1.81	0.45
1:B:252:ILE:O	1:B:252:ILE:HD12	2.16	0.45
1:E:109:LYS:HE2	1:E:123:VAL:HG13	1.99	0.45
1:D:157:LEU:HD11	1:F:81:ARG:HB3	1.99	0.45
1:D:204:HIS:CD2	1:E:207:PHE:CE2	3.05	0.45
1:A:93:LEU:HD23	1:A:93:LEU:N	2.32	0.45
1:B:121:HIS:CE1	1:B:227:GLY:O	2.70	0.45
1:D:236:LEU:HG	1:D:262:ILE:HD12	1.98	0.45
1:E:45:LEU:HD21	1:E:64:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:THR:HA	1:D:163:GLU:O	2.17	0.44
1:D:242:THR:HG22	1:D:268:ILE:CD1	2.46	0.44
1:E:277:ILE:HB	1:E:315:LEU:HD13	2.00	0.44
1:C:282:LEU:HD11	1:C:325:VAL:HG22	1.99	0.44
1:D:139:ASN:CB	2:E:345:GOL:H31	2.47	0.44
1:D:195:TYR:O	1:D:213:GLY:HA3	2.17	0.44
1:E:259:GLY:O	1:E:275:ARG:HA	2.17	0.44
1:A:129:PHE:HB2	1:A:130:PRO:HD3	1.99	0.44
1:A:182:VAL:HG22	1:A:196:ILE:HG22	1.99	0.44
1:B:270:ILE:CD1	1:B:305:ALA:HB1	2.48	0.44
1:B:174[A]:THR:CG2	1:B:187:THR:HB	2.48	0.44
1:B:222:GLY:HA3	1:B:240:CYS:SG	2.58	0.44
1:F:252:ILE:O	1:F:252:ILE:CD1	2.65	0.44
1:F:94:LEU:CD1	1:F:108:LEU:HD23	2.48	0.43
1:C:182:VAL:CG2	1:C:196:ILE:HG22	2.48	0.43
1:C:311:GLN:HB2	1:C:314:LEU:HD11	2.00	0.43
1:B:87:LYS:NZ	3:B:358:HOH:O	2.45	0.43
1:F:16:ASN:HD21	1:F:20:ALA:HB3	1.83	0.43
1:B:293:LEU:HD23	1:B:299:LEU:HA	2.01	0.43
1:F:107:TYR:O	1:F:111:HIS:ND1	2.46	0.43
1:A:301:LYS:HG3	1:A:303:VAL:HG13	2.01	0.43
1:C:286:ALA:HB1	1:C:306:ARG:CZ	2.49	0.43
1:C:5:LEU:HD12	1:C:38:VAL:HG21	2.00	0.43
1:D:252:ILE:CD1	1:D:252:ILE:O	2.67	0.43
1:D:3:GLN:NE2	1:D:95:ALA:HB1	2.34	0.43
1:C:64:LEU:CB	1:C:79:LEU:HD13	2.49	0.43
1:E:300:VAL:HG12	1:E:301:LYS:HG2	2.00	0.43
1:F:314:LEU:CD2	1:F:329:THR:HG22	2.49	0.43
1:A:174[B]:THR:HG21	1:A:187:THR:CB	2.49	0.42
1:A:302:VAL:HG11	1:C:321:GLN:NE2	2.34	0.42
1:C:57:THR:HG23	1:C:60:GLN:H	1.84	0.42
1:D:64:LEU:HB3	1:D:79:LEU:HD13	2.01	0.42
1:F:168:ASP:OD1	1:F:169:LYS:N	2.48	0.42
1:F:203:MET:HB2	1:F:221:GLU:HG2	2.01	0.42
1:A:5:LEU:HD12	1:A:38:VAL:CG2	2.49	0.42
1:B:41:VAL:CG1	1:B:45:LEU:HD12	2.50	0.42
1:D:242:THR:HA	1:D:268:ILE:HG12	2.01	0.42
1:A:268:ILE:HG21	1:A:272:LEU:HD11	2.01	0.42
1:C:57:THR:HG23	1:C:59:GLN:H	1.83	0.42
1:D:14:THR:HG23	1:D:23:GLU:HG3	2.01	0.42
1:E:15:GLN:HE21	1:E:88:PRO:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HA	1:C:92:THR:O	2.20	0.42
1:E:42:ALA:HB3	1:E:43:PRO:HD3	2.01	0.42
1:E:57[A]:THR:HG22	3:E:378:HOH:O	2.20	0.42
1:F:59:GLN:HE21	1:F:59:GLN:N	2.18	0.41
1:C:58:SER:OG	1:C:83:ALA:O	2.38	0.41
1:E:195:TYR:O	1:E:213:GLY:HA3	2.20	0.41
1:D:8:LEU:HD23	1:D:33:PRO:CB	2.51	0.41
1:E:135:VAL:HG11	1:E:142:ALA:HB1	2.02	0.41
1:A:8:LEU:C	1:A:8:LEU:HD12	2.41	0.41
1:C:270:ILE:HD13	1:C:305:ALA:HB1	2.03	0.41
1:D:58:SER:OG	1:D:83:ALA:O	2.26	0.41
1:E:268:ILE:HD12	1:E:272:LEU:HG	2.03	0.41
1:B:128:ILE:HG23	1:B:129:PHE:HD1	1.85	0.41
1:B:64:LEU:HB3	1:B:79:LEU:HD13	2.03	0.41
1:D:168:ASP:OD1	1:F:183:ARG:HD2	2.21	0.41
1:F:129:PHE:O	1:F:169:LYS:NZ	2.52	0.41
1:E:268:ILE:HG21	1:E:272:LEU:HD11	2.03	0.40
2:E:345:GOL:H12	1:F:139:ASN:CB	2.51	0.40
1:D:204:HIS:H	1:D:204:HIS:CD2	2.40	0.40
1:A:15:GLN:HE21	1:A:88:PRO:HG3	1.86	0.40
1:D:141:GLY:HA2	3:D:664:HOH:O	2.20	0.40
1:E:174:THR:CG2	1:E:178:VAL:HG22	2.42	0.40
1:E:252:ILE:O	1:E:252:ILE:HD12	2.22	0.40
1:A:5:LEU:HD12	1:A:38:VAL:HG22	2.03	0.40
1:B:270:ILE:HD13	1:B:305:ALA:HB1	2.03	0.40
1:E:182:VAL:HG11	1:E:196:ILE:CG2	2.51	0.40
1:F:15:GLN:HB3	1:F:19:GLU:HA	2.02	0.40
1:A:182:VAL:CG2	1:A:196:ILE:HG22	2.52	0.40
1:B:220:ILE:HD13	1:B:236:LEU:HD13	2.04	0.40
1:E:136:ALA:HB2	1:E:145:LEU:CD2	2.49	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	316/347 (91%)	309 (98%)	7 (2%)	0	100	100
1	B	316/347 (91%)	312 (99%)	4 (1%)	0	100	100
1	C	314/347 (90%)	307 (98%)	7 (2%)	0	100	100
1	D	316/347 (91%)	310 (98%)	6 (2%)	0	100	100
1	E	316/347 (91%)	309 (98%)	7 (2%)	0	100	100
1	F	315/347 (91%)	309 (98%)	6 (2%)	0	100	100
All	All	1893/2082 (91%)	1856 (98%)	37 (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	245/263 (93%)	235 (96%)	10 (4%)	37	19
1	B	245/263 (93%)	239 (98%)	6 (2%)	57	41
1	C	244/263 (93%)	234 (96%)	10 (4%)	37	19
1	D	245/263 (93%)	239 (98%)	6 (2%)	57	41
1	E	245/263 (93%)	236 (96%)	9 (4%)	41	23
1	F	244/263 (93%)	235 (96%)	9 (4%)	41	23
All	All	1468/1578 (93%)	1418 (97%)	50 (3%)	44	26

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	59	GLN
1	A	66	ASP
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	135	VAL
1	A	182	VAL
1	A	261	LEU
1	A	297	ASN
1	A	317	ARG
1	A	319	ASN
1	B	8	LEU
1	B	18	GLN
1	B	243	MET
1	B	261	LEU
1	B	297	ASN
1	B	317	ARG
1	C	8	LEU
1	C	66	ASP
1	C	90	VAL
1	C	135	VAL
1	C	138	THR
1	C	251	ASN
1	C	261	LEU
1	C	297	ASN
1	C	306	ARG
1	C	317	ARG
1	D	8	LEU
1	D	14	THR
1	D	251	ASN
1	D	268	ILE
1	D	306	ARG
1	D	317	ARG
1	E	8	LEU
1	E	14	THR
1	E	57[A]	THR
1	E	57[B]	THR
1	E	66	ASP
1	E	93	LEU
1	E	297	ASN
1	E	306	ARG
1	E	317	ARG
1	F	8	LEU
1	F	14	THR
1	F	123	VAL
1	F	251	ASN
1	F	268	ILE

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Mol	Chain	Res	Type
1	F	297	ASN
1	F	306	ARG
1	F	317	ARG
1	F	319	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	52	GLN
1	A	60	GLN
1	A	115	HIS
1	A	134	ASN
1	A	251	ASN
1	A	276	ASN
1	A	319	ASN
1	B	15	GLN
1	B	52	GLN
1	B	60	GLN
1	B	115	HIS
1	B	121	HIS
1	B	134	ASN
1	B	204	HIS
1	B	251	ASN
1	B	276	ASN
1	B	319	ASN
1	B	321	GLN
1	C	15	GLN
1	C	52	GLN
1	C	115	HIS
1	C	121	HIS
1	C	134	ASN
1	C	204	HIS
1	C	276	ASN
1	C	319	ASN
1	C	321	GLN
1	D	3	GLN
1	D	52	GLN
1	D	60	GLN
1	D	115	HIS
1	D	121	HIS
1	D	134	ASN

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Mol	Chain	Res	Type
1	D	204	HIS
1	D	251	ASN
1	D	276	ASN
1	D	319	ASN
1	E	15	GLN
1	E	52	GLN
1	E	60	GLN
1	E	115	HIS
1	E	121	HIS
1	E	134	ASN
1	E	251	ASN
1	E	265	ASN
1	E	297	ASN
1	E	319	ASN
1	F	52	GLN
1	F	59	GLN
1	F	60	GLN
1	F	115	HIS
1	F	121	HIS
1	F	134	ASN
1	F	204	HIS
1	F	297	ASN
1	F	319	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

2 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	A	345	-	5,5,5	0.47	0	5,5,5	1.32	1 (20%)
2	GOL	E	345	-	5,5,5	0.38	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
2	GOL	A	345	-	-	0/4/4/4	0/0/0/0
2	GOL	E	345	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	345	GOL	O2-C2-C1	2.32	119.59	108.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	345	GOL	2	0
2	E	345	GOL	4	0

## 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, 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	320/347 (92%)	0.42	20 (6%) 23 19	13, 23, 49, 51	0
1	B	320/347 (92%)	0.54	37 (11%) 6 5	14, 23, 49, 51	0
1	C	319/347 (91%)	0.38	19 (5%) 25 20	14, 24, 48, 51	0
1	D	320/347 (92%)	0.40	25 (7%) 16 12	13, 22, 49, 52	0
1	E	320/347 (92%)	0.48	34 (10%) 8 6	13, 22, 48, 52	0
1	F	320/347 (92%)	0.37	22 (6%) 20 16	13, 23, 48, 51	0
All	All	1919/2082 (92%)	0.43	157 (8%) 14 11	13, 23, 48, 52	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	252	ILE	6.1
1	E	298	ALA	6.0
1	B	252	ILE	6.0
1	E	252	ILE	5.8
1	D	321	GLN	5.8
1	C	252	ILE	5.5
1	B	298	ALA	5.3
1	B	299	LEU	5.1
1	E	302	VAL	5.1
1	E	294	ASP	5.1
1	C	251	ASN	5.1
1	B	3	GLN	4.8
1	E	283	TYR	4.8
1	A	252	ILE	4.7
1	B	297	ASN	4.6
1	C	86	GLN	4.5
1	A	321	GLN	4.4
1	B	320	SER	4.4
1	D	320	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	294	ASP	4.3
1	A	302	VAL	4.3
1	B	302	VAL	4.3
1	A	298	ALA	4.2
1	F	251	ASN	4.2
1	D	252	ILE	4.2
1	E	297	ASN	4.1
1	D	298	ALA	4.1
1	E	244	GLY	4.1
1	A	320	SER	4.1
1	E	3	GLN	4.1
1	E	287	GLY	4.1
1	C	253	VAL	4.0
1	E	324	ALA	4.0
1	B	244	GLY	3.9
1	A	297	ASN	3.9
1	E	299	LEU	3.9
1	B	323	GLY	3.9
1	B	251	ASN	3.9
1	E	329	THR	3.7
1	C	3	GLN	3.7
1	A	3	GLN	3.6
1	B	321	GLN	3.6
1	B	293	LEU	3.6
1	E	300	VAL	3.6
1	C	18	GLN	3.5
1	B	295	GLU	3.5
1	E	295	GLU	3.5
1	D	319	ASN	3.4
1	E	251	ASN	3.4
1	E	323	GLY	3.4
1	A	325	VAL	3.4
1	F	18	GLN	3.3
1	A	299	LEU	3.3
1	D	297	ASN	3.3
1	D	299	LEU	3.3
1	D	323	GLY	3.2
1	A	322	ASN	3.2
1	B	303	VAL	3.2
1	A	251	ASN	3.2
1	D	283	TYR	3.1
1	D	251	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	324	ALA	3.1
1	B	308	LEU	3.0
1	D	302	VAL	3.0
1	A	300	VAL	3.0
1	F	297	ASN	2.9
1	E	12	VAL	2.9
1	E	320	SER	2.9
1	F	295	GLU	2.9
1	B	12	VAL	2.9
1	F	3	GLN	2.8
1	A	4	SER	2.8
1	D	69	LYS	2.8
1	B	283	TYR	2.8
1	F	4	SER	2.8
1	E	321	GLN	2.8
1	E	322	ASN	2.7
1	A	17	ARG	2.7
1	B	300	VAL	2.7
1	C	243	MET	2.7
1	F	294	ASP	2.7
1	C	49	ALA	2.7
1	F	86	GLN	2.7
1	E	301	LYS	2.7
1	A	86	GLN	2.7
1	D	17	ARG	2.7
1	E	10	PHE	2.6
1	B	269	GLY	2.6
1	F	17	ARG	2.6
1	F	244	GLY	2.6
1	F	321	GLN	2.6
1	C	61	ALA	2.6
1	C	321	GLN	2.6
1	D	3	GLN	2.6
1	A	69	LYS	2.6
1	B	24	VAL	2.6
1	D	325	VAL	2.6
1	B	305	ALA	2.5
1	C	297	ASN	2.5
1	B	243	MET	2.5
1	D	66	ASP	2.5
1	D	322	ASN	2.5
1	B	291	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	294	ASP	2.5
1	F	20	ALA	2.5
1	C	59	GLN	2.5
1	B	9	ALA	2.5
1	D	92[A]	THR	2.5
1	B	301	LYS	2.4
1	A	294	ASP	2.4
1	C	19	GLU	2.4
1	F	243	MET	2.4
1	D	4	SER	2.4
1	B	287	GLY	2.4
1	D	243	MET	2.4
1	C	329	THR	2.4
1	A	283	TYR	2.4
1	E	243	MET	2.4
1	F	59	GLN	2.4
1	D	307	ASP	2.3
1	B	325	VAL	2.3
1	E	90	VAL	2.3
1	C	48	ALA	2.3
1	B	329	THR	2.3
1	F	62	TYR	2.3
1	C	66	ASP	2.3
1	F	69	LYS	2.3
1	D	300	VAL	2.3
1	F	327	CYS	2.3
1	A	295	GLU	2.3
1	F	70	GLY	2.3
1	B	73	ALA	2.3
1	B	309	ALA	2.3
1	E	305	ALA	2.3
1	C	70	GLY	2.2
1	E	24	VAL	2.2
1	C	295	GLU	2.2
1	E	26	TYR	2.2
1	E	307	ASP	2.2
1	D	18	GLN	2.2
1	B	322	ASN	2.2
1	B	285	THR	2.2
1	B	10	PHE	2.2
1	F	309	ALA	2.2
1	F	316	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	303	VAL	2.2
1	E	293	LEU	2.2
1	A	9	ALA	2.1
1	B	275	ARG	2.1
1	F	19	GLU	2.1
1	C	316	PHE	2.1
1	D	303	VAL	2.1
1	B	8	LEU	2.1
1	E	9	ALA	2.0
1	E	292	LEU	2.0
1	E	253	VAL	2.0
1	E	11	GLY	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 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	345	6/6	0.69	0.30	15.26	19,20,23,23	0
2	GOL	E	345	6/6	0.73	0.23	7.55	25,27,27,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.