



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 03:40 PM EDT

PDB ID : 3UGJ  
Title : Formyl Glycinamide ribonucleotide amidotransferase from *Salmonella Typhimurum*: Role of the ATP complexation and glutaminase domain in catalytic coupling  
Authors : Morar, M.; Tanwar, A.S.; Panjikar, S.; Anand, R.  
Deposited on : unknown  
Resolution : 1.78 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

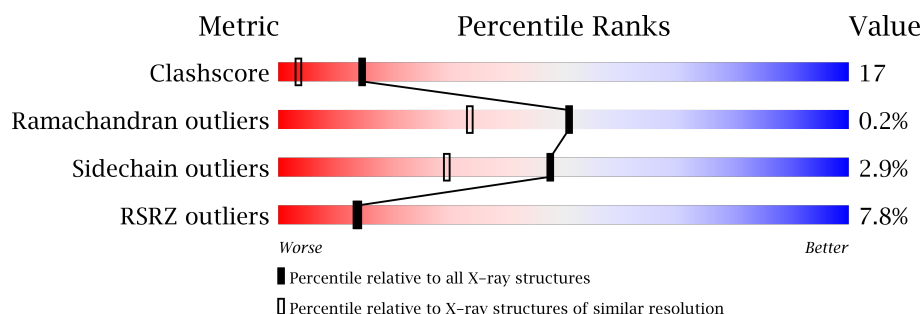
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	1303	<div> <div>8%</div> <div>72%</div> <div>25%</div> <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	SO4	A	2002	-	-	-	X
2	SO4	A	2009	-	-	-	X
3	ADP	A	2005	-	-	-	X
4	MG	A	2006	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	2007	-	-	-	X
4	MG	A	2008	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10759 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.

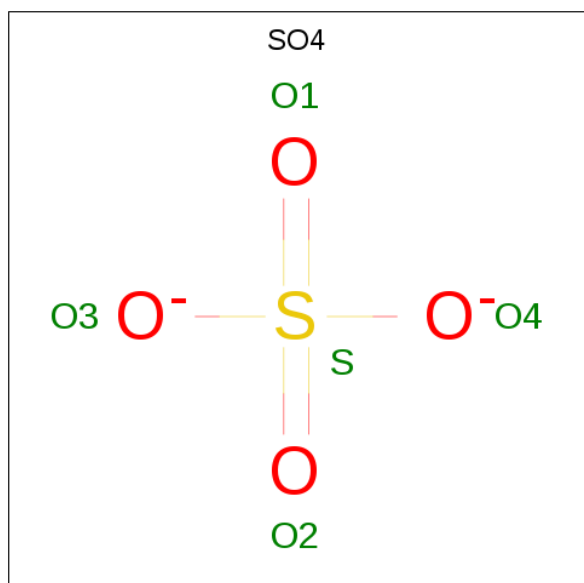
- Molecule 1 is a protein called Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1284	9884	6203	1766	1867	48	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

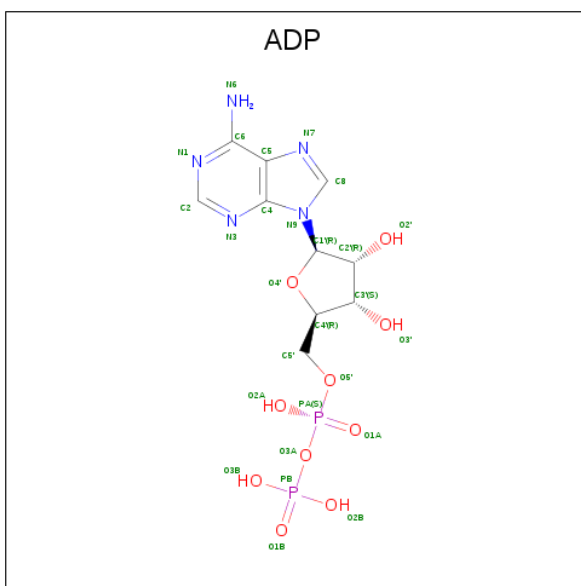
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P74881
A	-6	LEU	-	EXPRESSION TAG	UNP P74881
A	-5	VAL	-	EXPRESSION TAG	UNP P74881
A	-4	PRO	-	EXPRESSION TAG	UNP P74881
A	-3	ARG	-	EXPRESSION TAG	UNP P74881
A	-2	GLY	-	EXPRESSION TAG	UNP P74881
A	-1	SER	-	EXPRESSION TAG	UNP P74881
A	0	HIS	-	EXPRESSION TAG	UNP P74881

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0

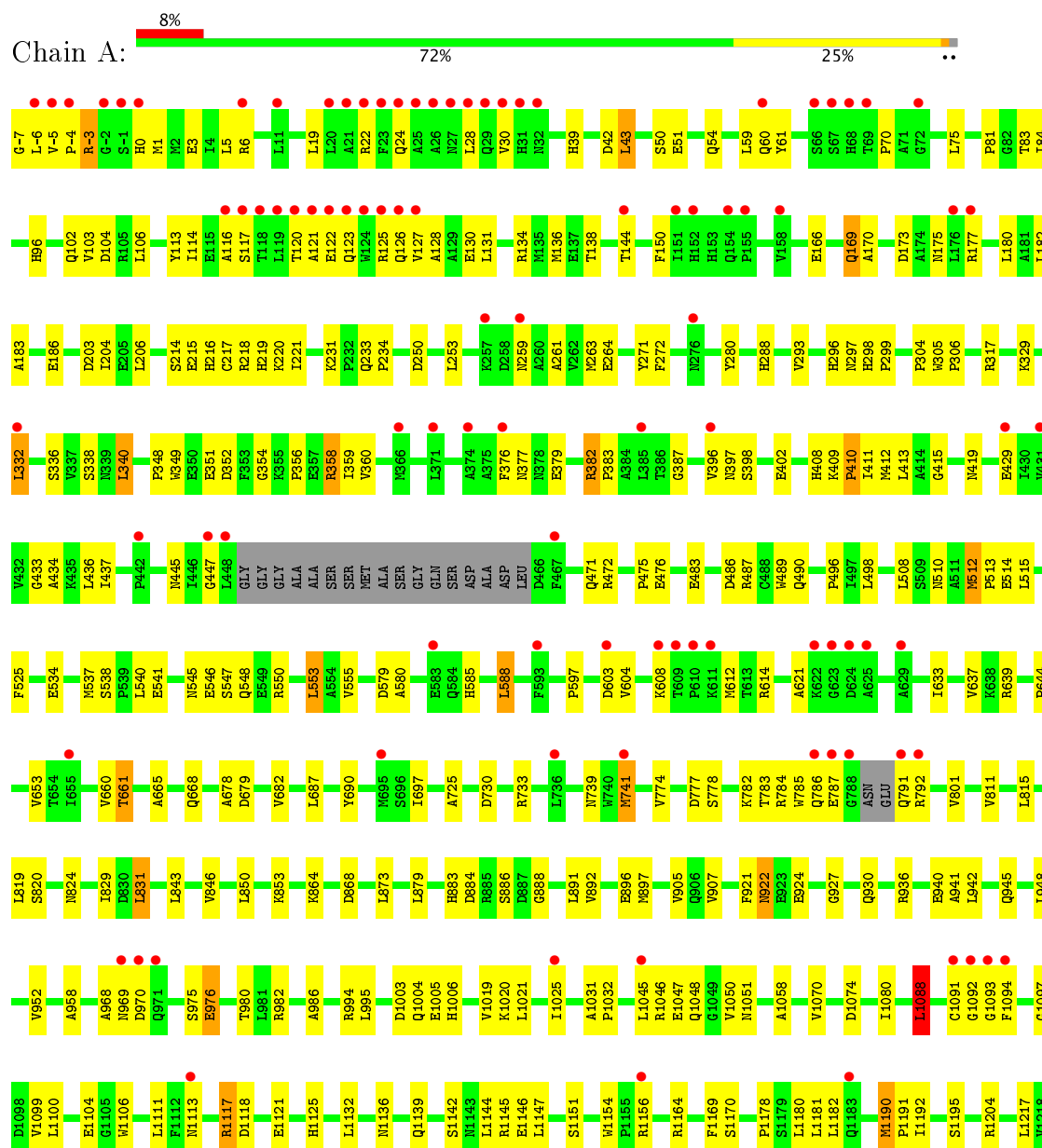
- Molecule 5 is water.

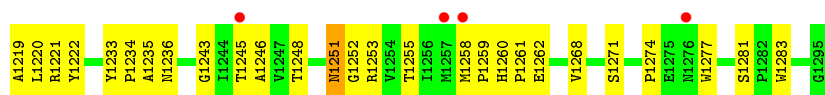
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	820	Total 820	O 820	0	0

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

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

- Molecule 1: Phosphoribosylformylglycinamide synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.98Å 145.98Å 141.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.78 47.78 – 1.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.78) 96.5 (47.78-1.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.211 , 0.240 0.214 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, 0.333 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: MG, SO4, ADP

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	0.34	1/10096 (0.0%)	0.64	3/13702 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1091	CYS	CB-SG	-6.45	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	LYS	N-CA-C	-5.94	94.96	111.00
1	A	1236	ASN	N-CA-C	-5.29	96.72	111.00
1	A	1088	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	9884	0	9675	335	0
2	A	25	0	0	0	0
3	A	27	0	12	1	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	820	0	0	85	0
All	All	10759	0	9687	336	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 17.

All (336) 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:358:ARG:HD3	1:A:358:ARG:H	1.06	1.12
1:A:340:LEU:HD11	1:A:644:PRO:HG2	1.38	1.05
1:A:261:ALA:HB2	1:A:774:VAL:HG13	1.39	1.02
1:A:639:ARG:HB3	1:A:846:VAL:HG21	1.38	1.00
1:A:1190:MET:H	1:A:1190:MET:HE2	1.30	0.97
1:A:1145:ARG:HD3	1:A:1154:TRP:HB2	1.48	0.94
1:A:358:ARG:CD	1:A:358:ARG:H	1.82	0.93
1:A:824:ASN:HD21	1:A:958:ALA:H	1.15	0.93
1:A:175:ASN:HD21	1:A:182:LEU:H	1.12	0.92
1:A:120:THR:HG23	1:A:123:GLN:HE21	1.35	0.91
1:A:653:VAL:HG22	5:A:2093:HOH:O	1.71	0.89
1:A:639:ARG:HB3	1:A:846:VAL:CG2	2.02	0.89
1:A:1178:PRO:HD2	5:A:2091:HOH:O	1.72	0.88
1:A:637:VAL:HG22	1:A:891:LEU:HD21	1.54	0.87
1:A:253:LEU:HD21	1:A:264:GLU:HG3	1.55	0.86
1:A:633:ILE:HG22	5:A:2064:HOH:O	1.75	0.85
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.41	0.85
1:A:358:ARG:HD3	1:A:358:ARG:N	1.90	0.84
1:A:-3:ARG:HD2	1:A:150:PHE:HB2	1.58	0.84
1:A:340:LEU:H	1:A:340:LEU:HD12	1.42	0.82
1:A:1111:LEU:HA	1:A:1117:ARG:HG3	1.62	0.81
1:A:1190:MET:N	1:A:1190:MET:HE2	1.96	0.81
1:A:534:GLU:HG3	1:A:537:MET:HG3	1.63	0.81
1:A:1217:LEU:HA	5:A:2091:HOH:O	1.81	0.80
1:A:733:ARG:HG2	5:A:2103:HOH:O	1.80	0.80
1:A:1178:PRO:HB2	5:A:2118:HOH:O	1.81	0.79
1:A:305:TRP:HB3	1:A:306:PRO:HD3	1.64	0.79
1:A:377:ASN:OD1	1:A:382:ARG:HD2	1.80	0.79
1:A:429:GLU:CD	1:A:429:GLU:H	1.85	0.78
1:A:922:ASN:HD22	1:A:924:GLU:H	1.32	0.77
1:A:820:SER:H	1:A:930:GLN:HE22	1.29	0.77
1:A:396:VAL:HG11	1:A:850:LEU:HD22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:CYS:HB2	5:A:1970:HOH:O	1.87	0.75
1:A:498:LEU:HD13	1:A:555:VAL:HA	1.67	0.75
1:A:1245:THR:HG23	5:A:1299:HOH:O	1.87	0.75
1:A:336:SER:HB2	1:A:411:ILE:HB	1.69	0.74
1:A:1070:VAL:HG22	1:A:1080:ILE:HD13	1.70	0.74
1:A:351:GLU:HG2	5:A:2071:HOH:O	1.89	0.72
1:A:905:VAL:HG13	1:A:907:VAL:HG13	1.70	0.72
1:A:665:ALA:CB	1:A:811:VAL:HG11	2.20	0.72
1:A:1222:TYR:OH	1:A:1245:THR:HG21	1.89	0.72
1:A:169:GLN:HE22	1:A:173:ASP:CG	1.93	0.72
1:A:545:ASN:HD22	1:A:547:SER:H	1.37	0.72
1:A:231:LYS:HG3	5:A:2072:HOH:O	1.88	0.71
1:A:1045:LEU:HG	1:A:1106:TRP:HZ2	1.56	0.71
1:A:1145:ARG:CD	1:A:1154:TRP:HB2	2.20	0.71
1:A:941:ALA:O	1:A:945:GLN:HG3	1.91	0.71
1:A:253:LEU:HD21	1:A:264:GLU:CG	2.21	0.71
1:A:261:ALA:HB2	1:A:774:VAL:CG1	2.18	0.70
1:A:843:LEU:O	1:A:846:VAL:HG12	1.91	0.70
1:A:1117:ARG:HD3	1:A:1147:LEU:HD11	1.72	0.70
1:A:1219:ALA:C	1:A:1220:LEU:HD22	2.12	0.70
1:A:348:PRO:HB2	5:A:1913:HOH:O	1.91	0.69
1:A:1252:GLY:HA2	5:A:2118:HOH:O	1.92	0.68
1:A:637:VAL:HG22	1:A:891:LEU:CD2	2.22	0.68
1:A:218:ARG:HD2	1:A:220:LYS:HG2	1.76	0.68
1:A:356:PRO:HG3	1:A:785:TRP:HB3	1.76	0.67
1:A:1004:GLN:NE2	1:A:1233:TYR:H	1.92	0.67
1:A:512:MET:HG3	1:A:525:PHE:CZ	2.30	0.67
1:A:1251:ASN:ND2	1:A:1253:ARG:H	1.92	0.67
1:A:639:ARG:HD3	5:A:1913:HOH:O	1.94	0.67
1:A:1156:ARG:HH21	1:A:1204:ARG:CZ	2.07	0.67
1:A:447:GLY:HA3	1:A:546:GLU:H	1.59	0.67
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.43	0.67
1:A:413:LEU:HD11	5:A:1941:HOH:O	1.95	0.66
1:A:175:ASN:ND2	1:A:182:LEU:H	1.92	0.66
1:A:19:LEU:HA	5:A:1972:HOH:O	1.96	0.66
1:A:5:LEU:HD22	1:A:59:LEU:HD12	1.76	0.65
1:A:447:GLY:CA	1:A:546:GLU:H	2.10	0.65
1:A:317:ARG:HH22	1:A:548:GLN:NE2	1.95	0.65
1:A:1220:LEU:HD23	1:A:1246:ALA:CB	2.27	0.64
1:A:221:ILE:HD13	1:A:612:MET:SD	2.37	0.64
1:A:739:ASN:HB2	5:A:1941:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HE1	1:A:103:VAL:O	1.80	0.64
1:A:261:ALA:CB	1:A:774:VAL:HG13	2.23	0.64
1:A:741:MET:HE2	1:A:778:SER:HB3	1.80	0.63
1:A:120:THR:HG23	1:A:123:GLN:NE2	2.09	0.63
1:A:383:PRO:HD3	1:A:660:VAL:HG13	1.79	0.63
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.00	0.63
1:A:183:ALA:HB3	1:A:186:GLU:HG3	1.80	0.63
1:A:483:GLU:OE1	1:A:487:ARG:NH2	2.31	0.63
1:A:349:TRP:HE3	5:A:1913:HOH:O	1.80	0.63
1:A:471:GLN:HE21	1:A:472:ARG:H	1.46	0.62
1:A:121:ALA:O	1:A:125:ARG:HD3	1.99	0.62
1:A:969:ASN:OD1	1:A:970:ASP:N	2.32	0.62
1:A:356:PRO:HG2	1:A:783:THR:CG2	2.30	0.62
1:A:976:GLU:HB3	5:A:1847:HOH:O	2.00	0.61
1:A:1245:THR:HG22	1:A:1259:PRO:HD3	1.82	0.61
1:A:127:VAL:HG12	5:A:2122:HOH:O	2.01	0.61
1:A:579:ASP:HB3	5:A:2104:HOH:O	2.00	0.61
1:A:332:LEU:HD13	1:A:415:GLY:C	2.21	0.61
1:A:733:ARG:N	5:A:2103:HOH:O	2.34	0.61
1:A:434:ALA:HB3	5:A:2120:HOH:O	2.00	0.60
1:A:682:VAL:HG11	1:A:811:VAL:HG13	1.83	0.60
1:A:1220:LEU:HB2	1:A:1246:ALA:HB3	1.83	0.60
1:A:791:GLN:HB3	5:A:2081:HOH:O	1.99	0.60
1:A:801:VAL:HB	5:A:1941:HOH:O	2.00	0.60
1:A:1156:ARG:HH21	1:A:1204:ARG:NH1	1.99	0.60
1:A:120:THR:OG1	1:A:123:GLN:HG3	2.01	0.60
1:A:1074:ASP:CB	1:A:1080:ILE:HD12	2.32	0.60
1:A:1:MET:HB3	5:A:2029:HOH:O	2.01	0.59
1:A:1219:ALA:O	1:A:1220:LEU:HD22	2.03	0.59
1:A:-3:ARG:HD3	1:A:42:ASP:OD1	2.03	0.59
1:A:218:ARG:HD2	1:A:220:LYS:CG	2.33	0.59
1:A:1051:ASN:H	1:A:1093:GLY:HA3	1.67	0.58
1:A:215:GLU:HA	5:A:1865:HOH:O	2.02	0.58
1:A:396:VAL:HG12	1:A:397:ASN:N	2.18	0.58
1:A:379:GLU:HB3	1:A:475:PRO:HB2	1.86	0.58
1:A:1220:LEU:HD23	1:A:1246:ALA:HB3	1.86	0.58
1:A:1117:ARG:HB3	1:A:1117:ARG:NH1	2.19	0.57
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.86	0.57
1:A:487:ARG:HH21	1:A:1046:ARG:NH2	2.02	0.57
1:A:1248:THR:HG23	5:A:2091:HOH:O	2.04	0.57
1:A:1113:ASN:HB3	5:A:1985:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLY:HA3	1:A:546:GLU:N	2.19	0.57
1:A:1190:MET:CE	1:A:1190:MET:N	2.68	0.57
1:A:298:HIS:HB3	1:A:299:PRO:HD3	1.85	0.57
1:A:396:VAL:HB	5:A:2050:HOH:O	2.05	0.57
1:A:1146:GLU:HG3	1:A:1147:LEU:HD13	1.87	0.57
1:A:1088:LEU:HD23	1:A:1088:LEU:C	2.25	0.56
1:A:792:ARG:HG3	5:A:2112:HOH:O	2.04	0.56
1:A:253:LEU:HD22	1:A:253:LEU:N	2.20	0.56
1:A:782:LYS:NZ	1:A:784:ARG:NH2	2.53	0.56
1:A:75:LEU:HD12	1:A:114:ILE:HD12	1.88	0.56
1:A:888:GLY:HA3	1:A:892:VAL:HG21	1.89	0.55
1:A:219:HIS:HD2	1:A:777:ASP:OD1	1.89	0.55
1:A:1169:PHE:CZ	1:A:1191:PRO:HB2	2.42	0.55
1:A:329:LYS:O	1:A:383:PRO:HD2	2.06	0.55
1:A:396:VAL:HG11	1:A:850:LEU:HB2	1.88	0.55
1:A:580:ALA:HB2	5:A:2120:HOH:O	2.06	0.55
1:A:1:MET:HE3	5:A:2029:HOH:O	2.06	0.55
1:A:515:LEU:HA	5:A:1989:HOH:O	2.05	0.54
1:A:1145:ARG:HD3	1:A:1154:TRP:CB	2.31	0.54
1:A:1255:THR:HB	5:A:2018:HOH:O	2.07	0.54
1:A:1117:ARG:HB3	1:A:1117:ARG:HH11	1.73	0.54
1:A:131:LEU:HD12	5:A:2122:HOH:O	2.07	0.54
1:A:668:GLN:HG2	5:A:2093:HOH:O	2.07	0.54
1:A:354:GLY:O	1:A:408:HIS:HE1	1.90	0.54
1:A:433:GLY:HA2	5:A:2104:HOH:O	2.07	0.54
1:A:1099:VAL:HG12	1:A:1100:LEU:HG	1.89	0.54
1:A:114:ILE:HD11	1:A:131:LEU:HD11	1.90	0.54
1:A:782:LYS:NZ	5:A:1428:HOH:O	2.40	0.54
1:A:-5:VAL:CG1	1:A:-4:PRO:HD2	2.37	0.53
1:A:1144:LEU:HD22	1:A:1147:LEU:HD22	1.91	0.53
1:A:510:ASN:O	1:A:514:GLU:HG3	2.09	0.53
1:A:6:ARG:HG2	5:A:1580:HOH:O	2.07	0.53
1:A:51:GLU:CD	1:A:102:GLN:HE22	2.12	0.53
1:A:1164:ARG:HD3	5:A:1350:HOH:O	2.08	0.53
1:A:-5:VAL:HB	5:A:2074:HOH:O	2.07	0.53
1:A:538:SER:OG	1:A:541:GLU:HG3	2.08	0.53
1:A:741:MET:CE	1:A:778:SER:HB3	2.38	0.53
1:A:122:GLU:O	1:A:126:GLN:HG3	2.09	0.52
1:A:398:SER:HB2	5:A:2050:HOH:O	2.08	0.52
1:A:483:GLU:O	1:A:487:ARG:HG2	2.08	0.52
1:A:639:ARG:CB	1:A:846:VAL:HG21	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:HIS:HD2	5:A:1529:HOH:O	1.91	0.52
1:A:774:VAL:HG12	5:A:1550:HOH:O	2.08	0.52
1:A:1222:TYR:CE2	1:A:1245:THR:OG1	2.57	0.52
1:A:349:TRP:CZ3	1:A:846:VAL:HG23	2.44	0.52
1:A:621:ALA:HA	5:A:2062:HOH:O	2.10	0.52
1:A:1271:SER:HA	5:A:2100:HOH:O	2.08	0.52
1:A:70:PRO:HB3	1:A:113:TYR:CE1	2.45	0.51
1:A:39:HIS:HD2	5:A:1458:HOH:O	1.92	0.51
1:A:-5:VAL:HG13	1:A:-4:PRO:HD2	1.92	0.51
1:A:639:ARG:NH1	5:A:1913:HOH:O	2.43	0.51
1:A:1251:ASN:HD22	1:A:1252:GLY:N	2.09	0.51
1:A:128:ALA:HA	5:A:2122:HOH:O	2.10	0.51
1:A:1178:PRO:O	1:A:1180:LEU:HD12	2.11	0.51
1:A:177:ARG:HG2	1:A:177:ARG:HH11	1.74	0.51
1:A:682:VAL:CG1	1:A:811:VAL:HG13	2.40	0.51
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.94	0.50
1:A:1005:GLU:HB2	1:A:1234:PRO:HD3	1.93	0.50
1:A:540:LEU:HD23	1:A:540:LEU:C	2.31	0.50
1:A:486:ASP:HA	1:A:489:TRP:NE1	2.27	0.50
1:A:508:LEU:CD1	1:A:550:ARG:NH1	2.74	0.50
1:A:220:LYS:HE3	5:A:1931:HOH:O	2.11	0.50
1:A:125:ARG:HD2	5:A:2046:HOH:O	2.11	0.50
1:A:358:ARG:CD	1:A:358:ARG:N	2.59	0.50
1:A:1146:GLU:HG2	5:A:1620:HOH:O	2.12	0.50
1:A:1222:TYR:CZ	1:A:1245:THR:HG21	2.46	0.50
1:A:815:LEU:HD13	1:A:879:LEU:HB2	1.93	0.50
1:A:994:ARG:HD2	1:A:1003:ASP:OD1	2.12	0.50
1:A:1074:ASP:HB3	1:A:1080:ILE:HD12	1.93	0.49
1:A:815:LEU:CD1	1:A:879:LEU:HD12	2.42	0.49
1:A:1006:HIS:HE1	5:A:1417:HOH:O	1.95	0.49
1:A:1180:LEU:HD13	1:A:1252:GLY:O	2.12	0.49
1:A:349:TRP:CE3	1:A:846:VAL:HG23	2.47	0.49
1:A:968:ALA:O	1:A:969:ASN:CG	2.50	0.49
1:A:1132:LEU:HA	5:A:2018:HOH:O	2.11	0.49
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.60	0.49
1:A:114:ILE:HD13	1:A:127:VAL:HG11	1.94	0.49
1:A:486:ASP:HA	1:A:489:TRP:CD1	2.47	0.49
1:A:665:ALA:CB	1:A:811:VAL:CG1	2.89	0.49
1:A:1025:ILE:HD11	1:A:1281:SER:HA	1.94	0.49
1:A:219:HIS:N	5:A:1854:HOH:O	2.46	0.49
1:A:447:GLY:N	1:A:546:GLU:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:HB3	5:A:1701:HOH:O	2.13	0.49
1:A:815:LEU:CD1	1:A:879:LEU:HB2	2.43	0.48
1:A:1180:LEU:HD13	1:A:1252:GLY:C	2.33	0.48
1:A:1181:LEU:HD12	5:A:2018:HOH:O	2.14	0.48
1:A:259:ASN:HB2	5:A:1404:HOH:O	2.14	0.48
1:A:948:LEU:O	1:A:952:VAL:HG23	2.13	0.48
1:A:402:GLU:HB2	5:A:1944:HOH:O	2.13	0.48
1:A:0:HIS:HB3	1:A:43:LEU:O	2.13	0.48
1:A:28:LEU:HD13	1:A:127:VAL:HG22	1.95	0.48
1:A:1192:ILE:HD13	1:A:1259:PRO:HB2	1.95	0.48
1:A:942:LEU:HD23	1:A:942:LEU:C	2.34	0.48
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.96	0.48
1:A:1121:GLU:O	1:A:1125:HIS:HD2	1.96	0.47
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.13	0.47
1:A:429:GLU:CD	1:A:429:GLU:N	2.60	0.47
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.13	0.47
1:A:220:LYS:HG3	5:A:1865:HOH:O	2.12	0.47
1:A:1104:GLU:HG3	5:A:1831:HOH:O	2.15	0.47
1:A:24:GLN:HB3	5:A:2057:HOH:O	2.14	0.47
1:A:545:ASN:ND2	1:A:547:SER:H	2.10	0.47
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.98	0.47
1:A:396:VAL:CG1	1:A:850:LEU:HB2	2.44	0.47
1:A:782:LYS:HE3	1:A:784:ARG:NH2	2.29	0.47
1:A:50:SER:O	1:A:54:GLN:HG3	2.15	0.47
1:A:668:GLN:NE2	5:A:2093:HOH:O	2.46	0.47
1:A:782:LYS:HZ1	1:A:784:ARG:NH2	2.13	0.47
1:A:508:LEU:HD13	1:A:550:ARG:NH1	2.30	0.47
1:A:1145:ARG:HH11	1:A:1145:ARG:HB3	1.79	0.47
1:A:1145:ARG:HD2	1:A:1151:SER:O	2.15	0.47
1:A:864:LYS:HE2	1:A:868:ASP:OD2	2.15	0.47
1:A:1259:PRO:O	1:A:1261:PRO:HD3	2.14	0.46
1:A:1047:GLU:HG3	1:A:1048:GLN:N	2.29	0.46
1:A:608:LYS:HA	5:A:1953:HOH:O	2.14	0.46
1:A:1245:THR:HG22	1:A:1258:MET:HB2	1.97	0.46
1:A:725:ALA:HB1	1:A:815:LEU:HB2	1.96	0.46
1:A:980:THR:HB	5:A:1847:HOH:O	2.14	0.46
1:A:668:GLN:HA	1:A:678:ALA:HB3	1.96	0.46
1:A:356:PRO:HD2	1:A:359:ILE:HD11	1.98	0.46
1:A:437:ILE:HB	1:A:553:LEU:HD23	1.98	0.46
1:A:175:ASN:ND2	1:A:180:LEU:HB2	2.20	0.45
1:A:-5:VAL:CG1	1:A:-4:PRO:CD	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HD3	1:A:138:THR:HG21	1.99	0.45
1:A:75:LEU:HD12	1:A:114:ILE:CD1	2.46	0.45
1:A:297:ASN:HB3	1:A:410:PRO:O	2.16	0.45
1:A:1251:ASN:ND2	1:A:1251:ASN:C	2.69	0.45
1:A:995:LEU:C	1:A:995:LEU:HD12	2.37	0.45
1:A:436:LEU:HD21	5:A:2120:HOH:O	2.17	0.45
1:A:376:PHE:CD1	1:A:475:PRO:HG3	2.52	0.45
1:A:1248:THR:CG2	5:A:2118:HOH:O	2.64	0.45
1:A:1190:MET:HE3	1:A:1283:TRP:CZ2	2.52	0.45
1:A:5:LEU:HD12	1:A:5:LEU:N	2.31	0.45
1:A:396:VAL:CG1	1:A:397:ASN:N	2.79	0.45
1:A:496:PRO:O	1:A:498:LEU:HD12	2.17	0.45
1:A:975:SER:O	1:A:976:GLU:HG2	2.17	0.45
1:A:288:HIS:O	1:A:419:ASN:HA	2.17	0.45
1:A:130:GLU:HG3	5:A:1921:HOH:O	2.17	0.44
1:A:515:LEU:HD23	1:A:515:LEU:C	2.37	0.44
1:A:387:GLY:HA2	1:A:697:ILE:HD12	1.99	0.44
1:A:922:ASN:ND2	1:A:924:GLU:H	2.08	0.44
1:A:123:GLN:O	1:A:127:VAL:HG23	2.18	0.44
1:A:1156:ARG:NH2	1:A:1204:ARG:NH1	2.63	0.44
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.53	0.44
1:A:891:LEU:HD23	1:A:921:PHE:CE1	2.52	0.44
1:A:1217:LEU:CD2	5:A:2091:HOH:O	2.66	0.44
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.82	0.44
1:A:396:VAL:CG1	1:A:850:LEU:HD22	2.41	0.44
1:A:873:LEU:CD2	1:A:942:LEU:HD13	2.48	0.44
1:A:1019:VAL:HG12	1:A:1020:LYS:N	2.33	0.44
1:A:166:GLU:HB2	1:A:170:ALA:HB2	1.99	0.43
1:A:356:PRO:HD2	1:A:359:ILE:CD1	2.48	0.43
1:A:585:HIS:HB3	5:A:2041:HOH:O	2.17	0.43
1:A:976:GLU:HG3	5:A:1879:HOH:O	2.17	0.43
1:A:1050:VAL:HG13	1:A:1092:GLY:O	2.17	0.43
1:A:1025:ILE:HD11	1:A:1281:SER:CA	2.48	0.43
1:A:1031:ALA:HB3	1:A:1032:PRO:HD3	2.00	0.43
1:A:665:ALA:HB3	1:A:811:VAL:HG11	1.98	0.43
1:A:-7:GLY:O	1:A:3:GLU:HG3	2.19	0.43
1:A:1019:VAL:CG1	1:A:1020:LYS:N	2.82	0.43
1:A:30:VAL:HA	1:A:116:ALA:HB2	2.00	0.43
1:A:1170:SER:O	1:A:1191:PRO:HA	2.19	0.43
1:A:1099:VAL:O	1:A:1100:LEU:HB2	2.18	0.42
1:A:338:SER:OG	1:A:408:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:TYR:CE1	1:A:1268:VAL:HG11	2.54	0.42
1:A:603:ASP:OD2	1:A:604:VAL:HG23	2.19	0.42
1:A:1245:THR:CG2	1:A:1259:PRO:HD3	2.48	0.42
1:A:633:ILE:C	5:A:2064:HOH:O	2.57	0.42
1:A:660:VAL:O	1:A:661:THR:HG23	2.19	0.42
1:A:787:GLU:HG2	1:A:792:ARG:CZ	2.48	0.42
1:A:304:PRO:HG3	1:A:360:VAL:HG21	2.00	0.42
1:A:687:LEU:HD13	1:A:1058:ALA:HB2	2.02	0.42
1:A:1004:GLN:HE21	1:A:1233:TYR:H	1.66	0.42
1:A:214:SER:N	5:A:1970:HOH:O	2.52	0.42
1:A:633:ILE:O	1:A:637:VAL:HG23	2.20	0.42
1:A:-6:LEU:HG	5:A:2029:HOH:O	2.20	0.42
1:A:936:ARG:O	1:A:940:GLU:HG3	2.19	0.42
1:A:-5:VAL:HG12	1:A:-4:PRO:N	2.34	0.42
1:A:1217:LEU:HD23	5:A:2091:HOH:O	2.19	0.42
1:A:352:ASP:C	5:A:2071:HOH:O	2.58	0.42
1:A:588:LEU:O	1:A:597:PRO:HD2	2.19	0.42
1:A:687:LEU:HD13	1:A:1058:ALA:CB	2.50	0.42
1:A:982:ARG:HH12	1:A:986:ALA:HB2	1.85	0.42
1:A:1094:PHE:HB3	1:A:1097:GLY:HA2	2.02	0.42
1:A:253:LEU:HD23	1:A:263:MET:C	2.40	0.42
1:A:340:LEU:HD11	1:A:644:PRO:CG	2.28	0.42
1:A:83:THR:HG22	1:A:84:ILE:N	2.35	0.42
1:A:853:LYS:HE2	5:A:2105:HOH:O	2.20	0.42
1:A:1142:SER:O	1:A:1145:ARG:HG3	2.20	0.41
1:A:332:LEU:HD22	1:A:332:LEU:O	2.19	0.41
1:A:786:GLN:HA	5:A:2112:HOH:O	2.20	0.41
1:A:829:ILE:HG22	1:A:831:LEU:HD13	2.02	0.41
1:A:103:VAL:HG11	1:A:106:LEU:HG	2.02	0.41
1:A:437:ILE:HB	1:A:553:LEU:CD2	2.49	0.41
1:A:819:LEU:HG	1:A:897:MET:HB3	2.02	0.41
1:A:436:LEU:CD2	5:A:2120:HOH:O	2.68	0.41
1:A:396:VAL:HG11	1:A:850:LEU:CD2	2.43	0.41
1:A:730:ASP:HB3	5:A:2103:HOH:O	2.20	0.41
1:A:1117:ARG:NH1	1:A:1118:ASP:OD1	2.54	0.41
3:A:2005:ADP:H1'	5:A:2093:HOH:O	2.20	0.41
1:A:498:LEU:N	1:A:498:LEU:HD12	2.35	0.41
1:A:884:ASP:HA	1:A:927:GLY:HA3	2.02	0.41
1:A:1234:PRO:O	1:A:1235:ALA:C	2.59	0.41
1:A:233:GLN:HA	1:A:234:PRO:HD3	1.86	0.41
1:A:272:PHE:CG	1:A:490:GLN:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:MET:HB3	1:A:513:PRO:HD3	2.02	0.41
1:A:741:MET:CE	1:A:778:SER:CB	2.99	0.41
1:A:1221:ARG:HA	1:A:1243:GLY:O	2.21	0.41
1:A:1190:MET:CE	1:A:1283:TRP:CZ2	3.03	0.41
1:A:1019:VAL:HG12	1:A:1021:LEU:HG	2.02	0.41
1:A:203:ASP:OD1	1:A:204:ILE:N	2.54	0.41
1:A:387:GLY:HA2	1:A:697:ILE:CD1	2.51	0.41
1:A:22:ARG:CZ	5:A:1972:HOH:O	2.69	0.40
1:A:782:LYS:CE	1:A:784:ARG:NH2	2.84	0.40
1:A:1121:GLU:O	1:A:1125:HIS:CD2	2.75	0.40
1:A:1274:PRO:HD2	1:A:1277:TRP:CE2	2.56	0.40
1:A:218:ARG:HB3	5:A:1865:HOH:O	2.20	0.40
1:A:668:GLN:CG	5:A:2093:HOH:O	2.68	0.40
1:A:134:ARG:HG2	5:A:1968:HOH:O	2.21	0.40
1:A:221:ILE:CD1	1:A:614:ARG:NH1	2.84	0.40
1:A:332:LEU:C	1:A:332:LEU:HD22	2.41	0.40
1:A:883:HIS:CE1	1:A:896:GLU:HB2	2.56	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	1278/1303 (98%)	1224 (96%)	51 (4%)	3 (0%)	51 33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	661	THR
1	A	886	SER

### 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	1028/1041 (99%)	998 (97%)	30 (3%)	48 29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	43	LEU
1	A	60	GLN
1	A	104	ASP
1	A	144	THR
1	A	169	GLN
1	A	206	LEU
1	A	250	ASP
1	A	296	HIS
1	A	332	LEU
1	A	340	LEU
1	A	358	ARG
1	A	382	ARG
1	A	410	PRO
1	A	412	MET
1	A	445	ASN
1	A	476	GLU
1	A	512	MET
1	A	553	LEU
1	A	588	LEU
1	A	741	MET
1	A	831	LEU
1	A	922	ASN
1	A	976	GLU
1	A	1088	LEU
1	A	1117	ARG
1	A	1182	LEU
1	A	1190	MET
1	A	1195	SER
1	A	1251	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	39	HIS
1	A	60	GLN
1	A	96	HIS
1	A	97	ASN
1	A	123	GLN
1	A	126	GLN
1	A	169	GLN
1	A	175	ASN
1	A	216	HIS
1	A	219	HIS
1	A	233	GLN
1	A	283	HIS
1	A	298	HIS
1	A	408	HIS
1	A	419	ASN
1	A	445	ASN
1	A	471	GLN
1	A	545	ASN
1	A	548	GLN
1	A	585	HIS
1	A	739	ASN
1	A	746	HIS
1	A	818	GLN
1	A	824	ASN
1	A	883	HIS
1	A	916	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1026	ASN
1	A	1053	HIS
1	A	1061	HIS
1	A	1084	ASN
1	A	1125	HIS
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	SO4	A	2001	-	4,4,4	0.36	0	6,6,6	0.05	0
2	SO4	A	2002	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	A	2003	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	A	2004	-	4,4,4	0.28	0	6,6,6	0.09	0
3	ADP	A	2005	4	25,29,29	0.95	1 (4%)	24,45,45	2.17	1 (4%)
2	SO4	A	2009	-	4,4,4	0.32	0	6,6,6	0.08	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	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2004	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2005	4	-	0/12/32/32	0/3/3/3
2	SO4	A	2009	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2005	ADP	O4'-C1'	2.53	1.44	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2005	ADP	N3-C2-N1	-10.03	120.12	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2005	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1284/1303 (98%)	0.51	100 (7%)	14 14	8, 15, 21, 48	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	8.4
1	A	788	GLY	8.1
1	A	121	ALA	7.0
1	A	117	SER	6.9
1	A	25	ALA	6.9
1	A	119	LEU	6.8
1	A	120	THR	5.9
1	A	27	ASN	5.7
1	A	969	ASN	5.2
1	A	24	GLN	5.2
1	A	122	GLU	5.1
1	A	-5	VAL	5.1
1	A	116	ALA	5.0
1	A	448	LEU	4.8
1	A	124	TRP	4.8
1	A	66	SER	4.7
1	A	29	GLN	4.6
1	A	152	HIS	4.6
1	A	28	LEU	4.4
1	A	21	ALA	4.4
1	A	624	ASP	4.3
1	A	30	VAL	4.3
1	A	125	ARG	4.2
1	A	609	THR	4.0
1	A	791	GLN	4.0
1	A	26	ALA	4.0
1	A	610	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1091	CYS	3.7
1	A	31	HIS	3.7
1	A	593	PHE	3.7
1	A	69	THR	3.6
1	A	126	GLN	3.6
1	A	429	GLU	3.6
1	A	177	ARG	3.6
1	A	467	PHE	3.5
1	A	154	GLN	3.5
1	A	-1	SER	3.5
1	A	970	ASP	3.5
1	A	127	VAL	3.4
1	A	786	GLN	3.4
1	A	67	SER	3.4
1	A	23	PHE	3.4
1	A	123	GLN	3.3
1	A	6	ARG	3.3
1	A	447	GLY	3.3
1	A	176	LEU	3.3
1	A	1045	LEU	3.2
1	A	431	VAL	3.1
1	A	787	GLU	2.9
1	A	608	LYS	2.9
1	A	22	ARG	2.9
1	A	32	ASN	2.9
1	A	68	HIS	2.9
1	A	622	LYS	2.9
1	A	1276	ASN	2.8
1	A	792	ARG	2.7
1	A	1025	ILE	2.7
1	A	-6	LEU	2.7
1	A	60	GLN	2.7
1	A	72	GLY	2.6
1	A	151	ILE	2.6
1	A	-4	PRO	2.6
1	A	376	PHE	2.6
1	A	603	ASP	2.5
1	A	332	LEU	2.5
1	A	-2	GLY	2.5
1	A	971	GLN	2.5
1	A	695	MET	2.4
1	A	0	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1093	GLY	2.4
1	A	625	ALA	2.4
1	A	155	PRO	2.4
1	A	371	LEU	2.3
1	A	366	MET	2.3
1	A	374	ALA	2.3
1	A	741	MET	2.3
1	A	611	LYS	2.3
1	A	20	LEU	2.2
1	A	1094	PHE	2.2
1	A	655	ILE	2.2
1	A	1245	THR	2.2
1	A	385	LEU	2.2
1	A	583	GLU	2.1
1	A	259	ASN	2.1
1	A	1113	ASN	2.1
1	A	1257	MET	2.1
1	A	1156	ARG	2.1
1	A	1258	MET	2.1
1	A	257	LYS	2.1
1	A	158	VAL	2.1
1	A	11	LEU	2.1
1	A	736	LEU	2.1
1	A	442	PRO	2.0
1	A	629	ALA	2.0
1	A	1183	GLN	2.0
1	A	1092	GLY	2.0
1	A	396	VAL	2.0
1	A	144	THR	2.0
1	A	276	ASN	2.0
1	A	623	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
3	ADP	A	2005	27/27	0.95	0.58	17.59	6,14,15,16	27
4	MG	A	2006	1/1	0.86	0.22	12.10	20,20,20,20	0
4	MG	A	2008	1/1	0.81	0.28	7.40	21,21,21,21	0
4	MG	A	2007	1/1	0.92	0.26	4.33	21,21,21,21	0
2	SO4	A	2009	5/5	0.96	0.15	3.70	39,40,40,42	0
2	SO4	A	2002	5/5	0.97	0.16	2.45	31,33,36,36	0
2	SO4	A	2003	5/5	0.86	0.20	1.83	38,40,41,42	0
2	SO4	A	2001	5/5	0.94	0.18	1.21	40,41,42,42	0
2	SO4	A	2004	5/5	0.98	0.15	0.64	33,34,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.