



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 05:12 PM EDT

PDB ID : 4ZCI / pdb_00004zci
Title : Crystal Structure of Escherichia coli GTPase BipA/TypA
Authors : Fan, H.T.; Hahm, J.; Diggs, S.; Blaha, G.
Deposited on : 2015-04-16
Resolution : 2.63 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

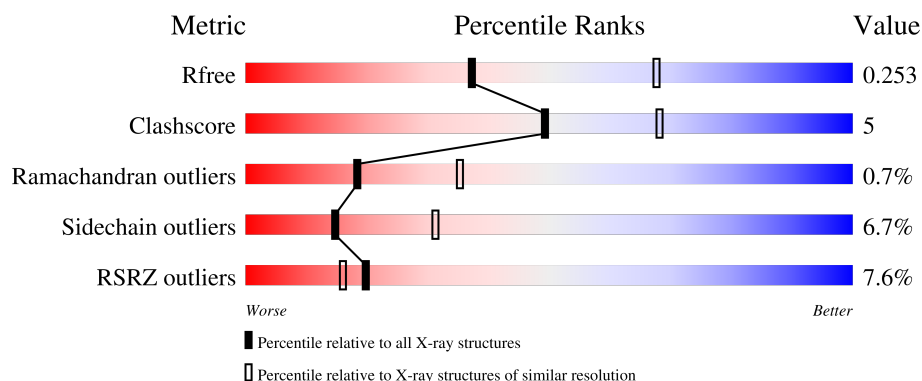
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	635	5% 71% 15% • 12%
1	B	635	9% 74% 13% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8661 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 GTP-binding protein TypA/BipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4315	2703	763	832	17			
1	B	561	Total	C	N	O	S	0	0	0
			4239	2658	753	811	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP P32132
A	-32	GLY	-	expression tag	UNP P32132
A	-31	SER	-	expression tag	UNP P32132
A	-30	SER	-	expression tag	UNP P32132
A	-29	HIS	-	expression tag	UNP P32132
A	-28	HIS	-	expression tag	UNP P32132
A	-27	HIS	-	expression tag	UNP P32132
A	-26	HIS	-	expression tag	UNP P32132
A	-25	HIS	-	expression tag	UNP P32132
A	-24	HIS	-	expression tag	UNP P32132
A	-23	SER	-	expression tag	UNP P32132
A	-22	SER	-	expression tag	UNP P32132
A	-21	GLY	-	expression tag	UNP P32132
A	-20	LEU	-	expression tag	UNP P32132
A	-19	VAL	-	expression tag	UNP P32132
A	-18	PRO	-	expression tag	UNP P32132
A	-17	ARG	-	expression tag	UNP P32132
A	-16	GLY	-	expression tag	UNP P32132
A	-15	SER	-	expression tag	UNP P32132
A	-14	HIS	-	expression tag	UNP P32132
A	-13	MET	-	expression tag	UNP P32132
A	-12	ALA	-	expression tag	UNP P32132
A	-11	SER	-	expression tag	UNP P32132
A	-10	MET	-	expression tag	UNP P32132
A	-9	THR	-	expression tag	UNP P32132

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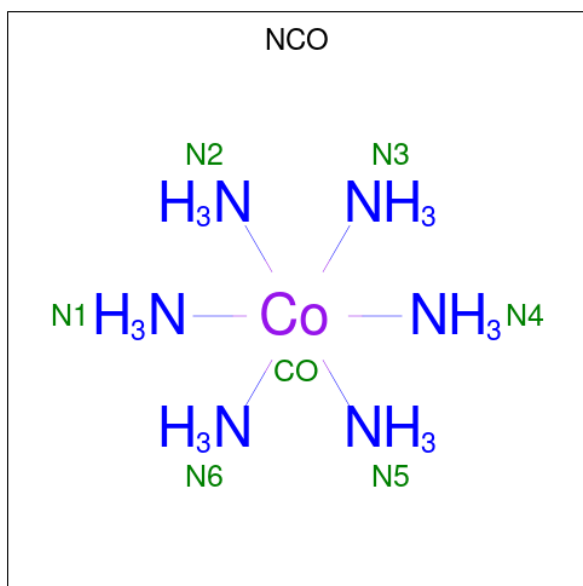
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P32132
A	-7	GLY	-	expression tag	UNP P32132
A	-6	GLN	-	expression tag	UNP P32132
A	-5	GLN	-	expression tag	UNP P32132
A	-4	MET	-	expression tag	UNP P32132
A	-3	GLY	-	expression tag	UNP P32132
A	-2	ARG	-	expression tag	UNP P32132
A	-1	GLY	-	expression tag	UNP P32132
A	0	SER	-	expression tag	UNP P32132
B	-33	MET	-	initiating methionine	UNP P32132
B	-32	GLY	-	expression tag	UNP P32132
B	-31	SER	-	expression tag	UNP P32132
B	-30	SER	-	expression tag	UNP P32132
B	-29	HIS	-	expression tag	UNP P32132
B	-28	HIS	-	expression tag	UNP P32132
B	-27	HIS	-	expression tag	UNP P32132
B	-26	HIS	-	expression tag	UNP P32132
B	-25	HIS	-	expression tag	UNP P32132
B	-24	HIS	-	expression tag	UNP P32132
B	-23	SER	-	expression tag	UNP P32132
B	-22	SER	-	expression tag	UNP P32132
B	-21	GLY	-	expression tag	UNP P32132
B	-20	LEU	-	expression tag	UNP P32132
B	-19	VAL	-	expression tag	UNP P32132
B	-18	PRO	-	expression tag	UNP P32132
B	-17	ARG	-	expression tag	UNP P32132
B	-16	GLY	-	expression tag	UNP P32132
B	-15	SER	-	expression tag	UNP P32132
B	-14	HIS	-	expression tag	UNP P32132
B	-13	MET	-	expression tag	UNP P32132
B	-12	ALA	-	expression tag	UNP P32132
B	-11	SER	-	expression tag	UNP P32132
B	-10	MET	-	expression tag	UNP P32132
B	-9	THR	-	expression tag	UNP P32132
B	-8	GLY	-	expression tag	UNP P32132
B	-7	GLY	-	expression tag	UNP P32132
B	-6	GLN	-	expression tag	UNP P32132
B	-5	GLN	-	expression tag	UNP P32132
B	-4	MET	-	expression tag	UNP P32132
B	-3	GLY	-	expression tag	UNP P32132
B	-2	ARG	-	expression tag	UNP P32132
B	-1	GLY	-	expression tag	UNP P32132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P32132

- Molecule 2 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		

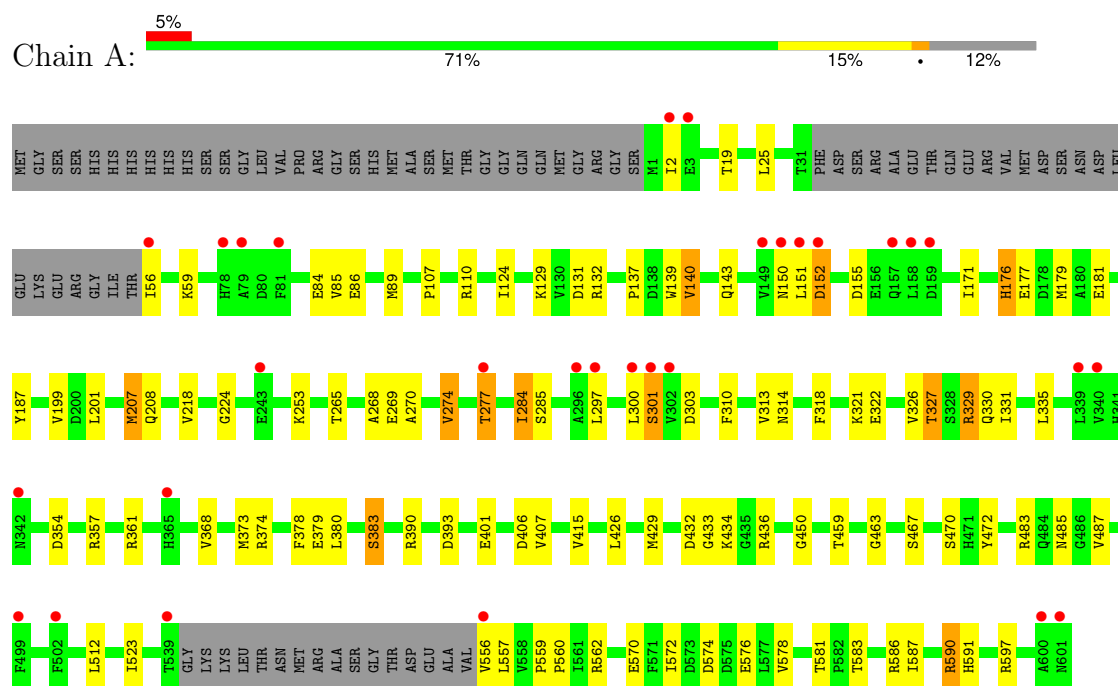
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	38	Total	O	0	0
			38	38		

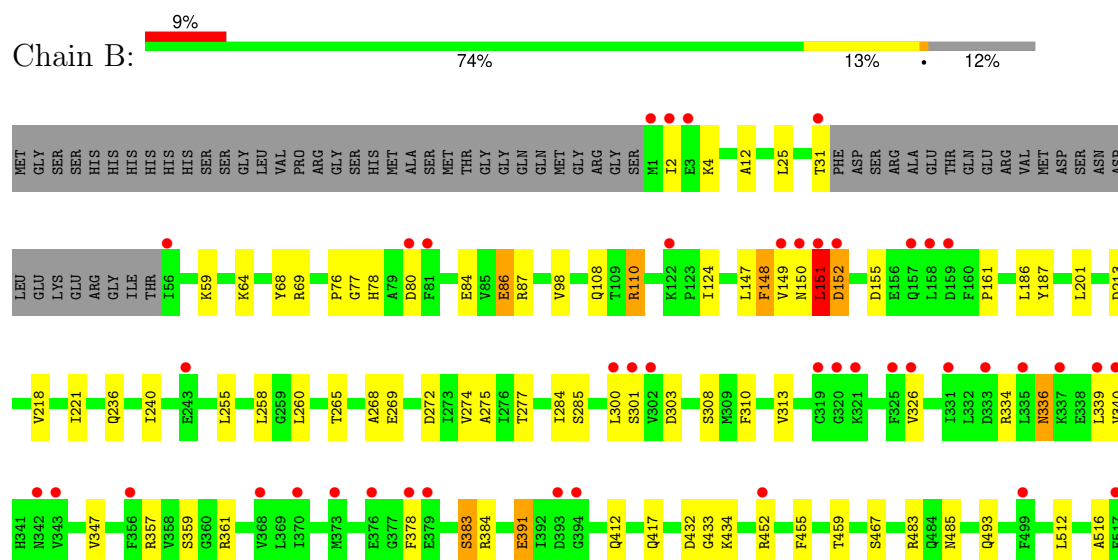
3 Residue-property plots

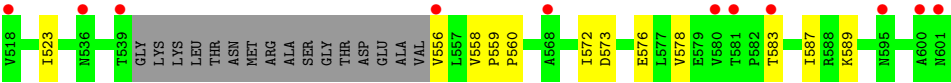
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GTP-binding protein TypA/BipA



• Molecule 1: GTP-binding protein TypA/BipA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.72Å 161.39Å 89.60Å 90.00° 97.95° 90.00°	Depositor
Resolution (Å)	46.00 – 2.63 46.00 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.00-2.63) 98.4 (46.00-2.63)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_1819	Depositor
R, R_{free}	0.210 , 0.248 0.220 , 0.253	Depositor DCC
R_{free} test set	2261 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8661	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/4383	0.75	2/5936 (0.0%)
1	B	0.31	0/4306	0.76	2/5839 (0.0%)
All	All	0.32	0/8689	0.76	4/11775 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASN	N-CA-C	-5.76	104.88	112.72
1	B	433	GLY	N-CA-C	-5.38	107.68	115.27
1	B	150	ASN	N-CA-C	-5.20	104.32	111.81
1	A	433	GLY	N-CA-C	-5.14	108.23	115.32

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	4315	0	4269	51	0
1	B	4239	0	4139	41	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
3	A	41	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	38	0	0	2	0
All	All	8661	0	8408	92	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 5.

All (92) 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:152:ASP:N	1:A:152:ASP:OD1	2.17	0.74
1:A:327:THR:HG23	1:A:329:ARG:H	1.59	0.67
1:B:255:LEU:HB2	1:B:275:ALA:HB3	1.79	0.65
1:A:407:VAL:HG11	1:A:415:VAL:HG21	1.81	0.62
1:A:326:VAL:HG12	1:A:379:GLU:HB3	1.81	0.62
1:B:149:VAL:O	1:B:149:VAL:HG22	2.00	0.61
1:A:277:THR:O	3:A:1101:HOH:O	2.16	0.61
1:B:572:ILE:HD13	1:B:578:VAL:HG23	1.81	0.61
1:A:137:PRO:HG2	1:A:176:HIS:ND1	2.18	0.58
1:B:147:LEU:C	1:B:149:VAL:H	2.11	0.57
1:A:379:GLU:HG3	1:A:581:THR:HG22	1.86	0.57
1:B:12:ALA:HB2	1:B:98:VAL:HB	1.86	0.57
1:B:417:GLN:NE2	3:B:1102:HOH:O	2.30	0.56
1:B:69:ARG:NH2	1:B:272:ASP:OD1	2.40	0.55
1:A:253:LYS:HD2	1:A:277:THR:HG21	1.90	0.54
1:B:25:LEU:O	1:B:187:TYR:OH	2.25	0.53
1:B:308:SER:HA	1:B:359:SER:HA	1.91	0.52
1:A:390:ARG:NH1	1:A:472:TYR:OH	2.41	0.52
1:A:176:HIS:CD2	1:A:177:GLU:HG3	2.46	0.51
1:A:426:LEU:HD21	1:A:429:MET:HE2	1.93	0.51
1:B:86:GLU:HG3	1:B:301:SER:HB2	1.92	0.51
1:A:450:GLY:O	1:A:570:GLU:HG3	2.10	0.51
1:B:4:LYS:HB3	1:B:68:TYR:HA	1.92	0.51
1:B:25:LEU:HD21	1:B:186:LEU:HD23	1.94	0.50
1:A:314:ASN:OD1	3:A:1102:HOH:O	2.20	0.50
1:B:523:ILE:HD12	1:B:587:ILE:HG22	1.93	0.50
1:B:110:ARG:NH1	1:B:467:SER:O	2.45	0.50
1:B:149:VAL:C	1:B:151:LEU:H	2.20	0.50
1:A:487:VAL:HG11	1:A:523:ILE:HD13	1.93	0.50
1:A:25:LEU:O	1:A:187:TYR:OH	2.27	0.49
1:B:236:GLN:NE2	3:B:1106:HOH:O	2.44	0.49
1:A:572:ILE:HD13	1:A:578:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:MET:O	1:A:378:PHE:HB2	2.13	0.49
1:A:313:VAL:HG22	1:A:354:ASP:HB3	1.95	0.48
1:A:556:VAL:HG23	1:A:557:LEU:HG	1.96	0.48
1:B:310:PHE:HB2	1:B:383:SER:HB3	1.96	0.48
1:A:591:HIS:HB2	1:A:597:ARG:HG2	1.96	0.47
1:B:268:ALA:HB1	1:B:274:VAL:HG11	1.96	0.47
1:B:301:SER:O	1:B:301:SER:OG	2.30	0.47
1:A:107:PRO:O	1:A:110:ARG:HB2	2.13	0.47
1:A:129:LYS:NZ	3:A:1105:HOH:O	2.48	0.47
1:B:391:GLU:O	1:B:391:GLU:HG3	2.15	0.47
1:A:139:TRP:HE3	1:A:140:VAL:HG12	1.79	0.47
1:A:318:PHE:HA	1:A:321:LYS:HD2	1.97	0.47
1:B:336:ASN:N	1:B:336:ASN:OD1	2.48	0.47
1:A:301:SER:O	1:A:301:SER:OG	2.31	0.46
1:A:523:ILE:HD12	1:A:587:ILE:HG22	1.98	0.46
1:B:334:ARG:HD3	1:B:378:PHE:HE2	1.80	0.46
1:A:151:LEU:HD11	1:A:470:SER:OG	2.16	0.46
1:A:483:ARG:HD2	1:A:485:ASN:O	2.16	0.45
1:B:147:LEU:O	1:B:149:VAL:N	2.42	0.45
1:B:64:LYS:HE3	1:B:258:LEU:HD11	1.97	0.45
1:A:574:ASP:O	1:A:590:ARG:NH1	2.50	0.45
1:B:432:ASP:HB3	1:B:434:LYS:H	1.81	0.45
1:B:77:GLY:O	1:B:78:HIS:ND1	2.49	0.44
1:B:76:PRO:HG2	1:B:84:GLU:HB3	1.99	0.44
1:A:139:TRP:O	1:A:143:GLN:HG2	2.18	0.43
1:B:576:GLU:HG2	1:B:589:LYS:HD3	1.99	0.43
1:A:85:VAL:O	1:A:89:MET:HG2	2.18	0.43
1:A:131:ASP:OD1	1:A:131:ASP:N	2.51	0.43
1:B:201:LEU:HD11	1:B:269:GLU:HB3	2.01	0.43
1:A:199:VAL:HB	1:A:270:ALA:HB1	2.01	0.43
1:A:432:ASP:HB3	1:A:434:LYS:H	1.83	0.43
1:A:207:MET:HE2	1:A:224:GLY:C	2.44	0.43
1:B:284:ILE:O	1:B:285:SER:HB2	2.19	0.43
1:A:401:GLU:OE1	1:A:467:SER:OG	2.27	0.42
1:A:268:ALA:HB1	1:A:274:VAL:HG11	2.01	0.42
1:A:331:ILE:O	1:A:335:LEU:HG	2.18	0.42
1:B:108:GLN:N	1:B:108:GLN:OE1	2.53	0.42
1:B:213:ASP:HB3	1:B:221:ILE:HB	2.01	0.42
1:B:339:LEU:HD21	1:B:347:VAL:HG23	2.01	0.42
1:B:124:ILE:HG23	1:B:161:PRO:HG2	2.00	0.41
1:A:322:GLU:OE1	1:A:586:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PHE:O	1:B:459:THR:HG22	2.21	0.41
1:A:310:PHE:HB2	1:A:383:SER:HB3	2.03	0.41
1:A:406:ASP:OD1	1:A:436:ARG:NE	2.39	0.41
1:B:483:ARG:HD2	1:B:485:ASN:O	2.21	0.41
1:A:374:ARG:HD2	1:A:581:THR:O	2.21	0.41
1:A:459:THR:CG2	1:A:463:GLY:H	2.34	0.41
1:A:559:PRO:HA	1:A:560:PRO:HD3	1.85	0.41
1:B:84:GLU:HA	1:B:87:ARG:HD2	2.03	0.41
1:B:148:PHE:HB3	1:B:152:ASP:OD2	2.20	0.41
1:B:452:ARG:HE	1:B:452:ARG:HB2	1.60	0.41
1:B:559:PRO:HA	1:B:560:PRO:HD3	1.74	0.41
1:A:483:ARG:NH1	1:A:576:GLU:OE1	2.54	0.40
1:A:208:GLN:HB2	1:A:297:LEU:HD12	2.03	0.40
1:A:201:LEU:HD11	1:A:269:GLU:HB3	2.03	0.40
1:B:334:ARG:HH11	1:B:334:ARG:HG2	1.86	0.40
1:A:284:ILE:O	1:A:285:SER:HB2	2.22	0.40
1:A:129:LYS:O	1:A:132:ARG:HG2	2.21	0.40
1:A:139:TRP:CE3	1:A:140:VAL:HG12	2.56	0.40
1:A:171:ILE:HG13	1:A:179:MET:HE3	2.04	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	555/635 (87%)	523 (94%)	30 (5%)	2 (0%)	30	49
1	B	555/635 (87%)	523 (94%)	26 (5%)	6 (1%)	11	23
All	All	1110/1270 (87%)	1046 (94%)	56 (5%)	8 (1%)	18	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	ASP
1	B	151	LEU
1	A	301	SER
1	B	516	ALA
1	A	2	ILE
1	B	148	PHE
1	B	2	ILE
1	B	326	VAL

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	466/540 (86%)	434 (93%)	32 (7%)	14	30
1	B	444/540 (82%)	415 (94%)	29 (6%)	15	33
All	All	910/1080 (84%)	849 (93%)	61 (7%)	15	31

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	56	ILE
1	A	59	LYS
1	A	84	GLU
1	A	86	GLU
1	A	124	ILE
1	A	140	VAL
1	A	152	ASP
1	A	155	ASP
1	A	176	HIS
1	A	181	GLU
1	A	207	MET
1	A	218	VAL
1	A	265	THR
1	A	274	VAL
1	A	277	THR

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Mol	Chain	Res	Type
1	A	284	ILE
1	A	300	LEU
1	A	303	ASP
1	A	327	THR
1	A	329	ARG
1	A	330	GLN
1	A	357	ARG
1	A	361	ARG
1	A	368	VAL
1	A	380	LEU
1	A	383	SER
1	A	393	ASP
1	A	512	LEU
1	A	562	ARG
1	A	583	THR
1	A	590	ARG
1	B	31	THR
1	B	59	LYS
1	B	86	GLU
1	B	110	ARG
1	B	151	LEU
1	B	152	ASP
1	B	155	ASP
1	B	218	VAL
1	B	240	ILE
1	B	260	LEU
1	B	265	THR
1	B	277	THR
1	B	300	LEU
1	B	303	ASP
1	B	313	VAL
1	B	336	ASN
1	B	340	VAL
1	B	357	ARG
1	B	361	ARG
1	B	383	SER
1	B	384	ARG
1	B	391	GLU
1	B	412	GLN
1	B	493	GLN
1	B	512	LEU
1	B	556	VAL

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Mol	Chain	Res	Type
1	B	558	VAL
1	B	573	ASP
1	B	583	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	60	ASN
1	A	71	ASN
1	A	176	HIS
1	A	208	GLN
1	A	342	ASN
1	B	293	ASN
1	B	342	ASN
1	B	372	ASN
1	B	484	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NCO	B	1002	-	6,6,6	0.49	0	-		
2	NCO	A	1001	-	6,6,6	0.51	0	-		
2	NCO	A	1002	-	6,6,6	0.49	0	-		
2	NCO	B	1001	-	6,6,6	0.50	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	561/635 (88%)	0.37	30 (5%)	32 27	35, 69, 121, 151	0
1	B	561/635 (88%)	0.60	55 (9%)	13 10	42, 75, 140, 179	0
All	All	1122/1270 (88%)	0.48	85 (7%)	20 16	35, 73, 133, 179	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	LEU	6.1
1	B	556	VAL	5.9
1	A	149	VAL	5.7
1	B	151	LEU	5.6
1	B	157	GLN	4.8
1	B	335	LEU	4.8
1	A	157	GLN	4.5
1	A	556	VAL	4.5
1	B	601	ASN	4.3
1	A	301	SER	3.9
1	B	158	LEU	3.9
1	B	149	VAL	3.9
1	B	243	GLU	3.8
1	B	499	PHE	3.7
1	A	601	ASN	3.6
1	B	302	VAL	3.6
1	B	301	SER	3.6
1	B	340	VAL	3.6
1	A	243	GLU	3.5
1	B	300	LEU	3.5
1	B	600	ALA	3.5
1	A	78	HIS	3.5
1	B	581	THR	3.4
1	B	373	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	PHE	3.2
1	B	333	ASP	3.1
1	A	151	LEU	3.1
1	A	539	THR	3.1
1	B	536	ASN	3.0
1	B	539	THR	3.0
1	A	302	VAL	2.9
1	B	150	ASN	2.9
1	A	340	VAL	2.9
1	A	277	THR	2.9
1	B	159	ASP	2.9
1	B	122	LYS	2.8
1	B	326	VAL	2.8
1	B	331	ILE	2.8
1	A	79	ALA	2.7
1	B	3	GLU	2.7
1	B	325	PHE	2.7
1	B	343	VAL	2.7
1	B	518	VAL	2.7
1	A	2	ILE	2.7
1	B	580	VAL	2.6
1	A	81	PHE	2.6
1	B	376	GLU	2.6
1	A	150	ASN	2.6
1	B	152	ASP	2.5
1	A	297	LEU	2.5
1	A	300	LEU	2.5
1	A	339	LEU	2.5
1	B	452	ARG	2.5
1	B	319	CYS	2.4
1	A	296	ALA	2.4
1	B	339	LEU	2.4
1	A	152	ASP	2.4
1	B	393	ASP	2.4
1	B	1	MET	2.4
1	B	81	PHE	2.4
1	B	370	ILE	2.4
1	A	3	GLU	2.4
1	B	80	ASP	2.3
1	B	394	GLY	2.3
1	B	368	VAL	2.3
1	B	517	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	31	THR	2.3
1	A	499	PHE	2.3
1	A	600	ALA	2.2
1	B	342	ASN	2.2
1	B	321	LYS	2.2
1	A	342	ASN	2.2
1	B	2	ILE	2.2
1	B	337	LYS	2.1
1	B	379	GLU	2.1
1	B	583	THR	2.1
1	B	595	ASN	2.1
1	A	56	ILE	2.1
1	B	568	ALA	2.1
1	B	320	GLY	2.1
1	B	56	ILE	2.0
1	A	502	PHE	2.0
1	B	356	PHE	2.0
1	A	159	ASP	2.0
1	A	365	HIS	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(Å ²)	Q<0.9
2	NCO	B	1002	7/7	0.92	0.12	107,110,112,112	0
2	NCO	A	1002	7/7	0.95	0.10	103,104,105,106	0
2	NCO	B	1001	7/7	0.98	0.09	61,66,69,70	0
2	NCO	A	1001	7/7	0.99	0.06	51,53,56,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.