

Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2022 – 06:39 pm GMT

PDB ID	:	7Q91
Title	:	Crystal Structure of Agrobacterium tumefaciens NADQ, native form.
Authors	:	Cianci, M.; Minazzato, G.; Heroux, A.; Raffaelli, N.; Sorci, L.; Gasparrini, M.
Deposited on	:	2021-11-11
Resolution	:	2.31 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.31 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	5974(2.34-2.30)		
Clashscore	141614	6604 (2.34-2.30)		
Ramachandran outliers	138981	6523 (2.34-2.30)		
Sidechain outliers	138945	6523 (2.34-2.30)		
RSRZ outliers	127900	$5855\ (2.34-2.30)$		

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 <=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	А	336	4%	7%	16%
1	В	336	13%	7%	18%
1	С	336	<u>6%</u> 75%	6%	20%
1	D	336	76%	6% •	18%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9271 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	281	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	201	2279	1445	415	415	4	0		
1	р	276	Total	С	Ν	0	S	0	0	0
	I D	270	2257	1432	414	407	4			
1	1 0	970	Total	С	Ν	0	S	0	0	0
	270	2196	1399	397	396	4	0	U	0	
1 D	275	Total	С	Ν	0	S	0	0	0	
		2230	1413	408	405	4		0	0	

• Molecule 1 is a protein called NADQ transcription factor.

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
А	-35	MET	-	initiating methionine	UNP A9CG24
А	-34	ARG	-	expression tag	UNP A9CG24
А	-33	GLY	-	expression tag	UNP A9CG24
А	-32	SER	-	expression tag	UNP A9CG24
А	-31	HIS	-	expression tag	UNP A9CG24
А	-30	HIS	-	expression tag	UNP A9CG24
А	-29	HIS	-	expression tag	UNP A9CG24
А	-28	HIS	-	expression tag	UNP A9CG24
А	-27	HIS	-	expression tag	UNP A9CG24
А	-26	HIS	-	expression tag	UNP A9CG24
A	-25	GLY	-	expression tag	UNP A9CG24
A	-24	MET	-	expression tag	UNP A9CG24
А	-23	ALA	-	expression tag	UNP A9CG24
A	-22	SER	-	expression tag	UNP A9CG24
А	-21	MET	-	expression tag	UNP A9CG24
A	-20	THR	-	expression tag	UNP A9CG24
A	-19	GLY	-	expression tag	UNP A9CG24
A	-18	GLY	-	expression tag	UNP A9CG24
A	-17	GLN	-	expression tag	UNP A9CG24
А	-16	GLN	-	expression tag	UNP A9CG24
А	-15	MET	-	expression tag	UNP A9CG24



Chain	Residue	Modelled	Actual Comment		Reference
А	-14	GLY	-	expression tag	UNP A9CG24
А	-13	ARG	-	expression tag	UNP A9CG24
А	-12	ASP	-	expression tag	UNP A9CG24
А	-11	LEU	-	expression tag	UNP A9CG24
А	-10	TYR	-	expression tag	UNP A9CG24
А	-9	ASP	-	expression tag	UNP A9CG24
А	-8	ASP	-	expression tag	UNP A9CG24
А	-7	ASP	-	expression tag	UNP A9CG24
А	-6	ASP	-	expression tag	UNP A9CG24
А	-5	LYS	-	expression tag	UNP A9CG24
А	-4	ASP	-	expression tag	UNP A9CG24
А	-3	HIS	-	expression tag	UNP A9CG24
А	-2	PRO	-	expression tag	UNP A9CG24
А	-1	PHE	-	expression tag	UNP A9CG24
А	0	THR	-	expression tag	UNP A9CG24
А	1	VAL	-	expression tag	UNP A9CG24
В	-35	MET	-	initiating methionine	UNP A9CG24
В	-34	ARG	-	expression tag	UNP A9CG24
В	-33	GLY	-	expression tag	UNP A9CG24
В	-32	SER	-	expression tag	UNP A9CG24
В	-31	HIS	-	expression tag	UNP A9CG24
В	-30	HIS	-	expression tag	UNP A9CG24
В	-29	HIS	-	expression tag	UNP A9CG24
В	-28	HIS	-	expression tag	UNP A9CG24
В	-27	HIS	-	expression tag	UNP A9CG24
В	-26	HIS	-	expression tag	UNP A9CG24
В	-25	GLY	-	expression tag	UNP A9CG24
В	-24	MET	-	expression tag	UNP A9CG24
В	-23	ALA	-	expression tag	UNP A9CG24
В	-22	SER	-	expression tag	UNP A9CG24
В	-21	MET	-	expression tag	UNP A9CG24
В	-20	THR	-	expression tag	UNP A9CG24
В	-19	GLY	-	expression tag	UNP A9CG24
В	-18	GLY	-	expression tag	UNP A9CG24
В	-17	GLN	-	expression tag	UNP A9CG24
В	-16	GLN	-	expression tag	UNP A9CG24
В	-15	MET	-	expression tag	UNP A9CG24
В	-14	GLY	-	expression tag	UNP A9CG24
В	-13	ARG	-	expression tag	UNP A9CG24
В	-12	ASP	-	expression tag	UNP A9CG24
В	-11	LEU	-	expression tag	UNP A9CG24
В	-10	TYR	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual Comment		Reference
В	-9	ASP	-	expression tag	UNP A9CG24
В	-8	ASP	-	expression tag	UNP A9CG24
В	-7	ASP	-	expression tag	UNP A9CG24
В	-6	ASP	-	expression tag	UNP A9CG24
В	-5	LYS	-	expression tag	UNP A9CG24
В	-4	ASP	-	expression tag	UNP A9CG24
В	-3	HIS	-	expression tag	UNP A9CG24
В	-2	PRO	-	expression tag	UNP A9CG24
В	-1	PHE	-	expression tag	UNP A9CG24
В	0	THR	-	expression tag	UNP A9CG24
В	1	VAL	-	expression tag	UNP A9CG24
С	-35	MET	-	initiating methionine	UNP A9CG24
С	-34	ARG	-	expression tag	UNP A9CG24
С	-33	GLY	-	expression tag	UNP A9CG24
С	-32	SER	-	expression tag	UNP A9CG24
С	-31	HIS	-	expression tag	UNP A9CG24
С	-30	HIS	-	expression tag	UNP A9CG24
С	-29	HIS	-	expression tag	UNP A9CG24
С	-28	HIS	-	expression tag	UNP A9CG24
С	-27	HIS	-	expression tag	UNP A9CG24
С	-26	HIS	-	expression tag	UNP A9CG24
С	-25	GLY	-	expression tag	UNP A9CG24
С	-24	MET	-	expression tag	UNP A9CG24
С	-23	ALA	-	expression tag	UNP A9CG24
С	-22	SER	-	expression tag	UNP A9CG24
С	-21	MET	-	expression tag	UNP A9CG24
С	-20	THR	-	expression tag	UNP A9CG24
С	-19	GLY	-	expression tag	UNP A9CG24
С	-18	GLY	-	expression tag	UNP A9CG24
С	-17	GLN	-	expression tag	UNP A9CG24
С	-16	GLN	-	expression tag	UNP A9CG24
С	-15	MET	-	expression tag	UNP A9CG24
С	-14	GLY	-	expression tag	UNP A9CG24
С	-13	ARG	-	expression tag	UNP A9CG24
С	-12	ASP	-	expression tag	UNP A9CG24
С	-11	LEU	-	expression tag	UNP A9CG24
С	-10	TYR	-	expression tag	UNP A9CG24
С	-9	ASP	-	expression tag	UNP A9CG24
C	-8	ASP	_	expression tag	UNP A9CG24
С	-7	ASP	-	expression tag	UNP A9CG24
C	-6	ASP	-	expression tag	UNP A9CG24
С	-5	LYS	-	expression tag	UNP A9CG24

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Chain	Residue	Modelled	Actual Comment		Reference
С	-4	ASP	-	expression tag	UNP A9CG24
С	-3	HIS	_	- expression tag	
С	-2	PRO	-	expression tag	UNP A9CG24
С	-1	PHE	-	expression tag	UNP A9CG24
С	0	THR	-	expression tag	UNP A9CG24
С	1	VAL	-	expression tag	UNP A9CG24
D	-35	MET	-	initiating methionine	UNP A9CG24
D	-34	ARG	-	expression tag	UNP A9CG24
D	-33	GLY	-	expression tag	UNP A9CG24
D	-32	SER	-	expression tag	UNP A9CG24
D	-31	HIS	-	expression tag	UNP A9CG24
D	-30	HIS	-	expression tag	UNP A9CG24
D	-29	HIS	-	expression tag	UNP A9CG24
D	-28	HIS	-	expression tag	UNP A9CG24
D	-27	HIS	-	expression tag	UNP A9CG24
D	-26	HIS	-	expression tag	UNP A9CG24
D	-25	GLY	-	expression tag	UNP A9CG24
D	-24	MET	-	expression tag	UNP A9CG24
D	-23	ALA	-	expression tag	UNP A9CG24
D	-22	SER	-	expression tag	UNP A9CG24
D	-21	MET	-	expression tag	UNP A9CG24
D	-20	THR	-	expression tag	UNP A9CG24
D	-19	GLY	-	expression tag	UNP A9CG24
D	-18	GLY	-	expression tag	UNP A9CG24
D	-17	GLN	-	expression tag	UNP A9CG24
D	-16	GLN	-	expression tag	UNP A9CG24
D	-15	MET	-	expression tag	UNP A9CG24
D	-14	GLY	-	expression tag	UNP A9CG24
D	-13	ARG	-	expression tag	UNP A9CG24
D	-12	ASP	-	expression tag	UNP A9CG24
D	-11	LEU	-	expression tag	UNP A9CG24
D	-10	TYR	-	expression tag	UNP A9CG24
D	-9	ASP	-	expression tag	UNP A9CG24
D	-8	ASP	-	expression tag	UNP A9CG24
D	-7	ASP	-	expression tag	UNP A9CG24
D	-6	ASP	-	expression tag	UNP A9CG24
D	-5	LYS	-	expression tag	UNP A9CG24
D	-4	ASP	-	expression tag	UNP A9CG24
D	-3	HIS	-	expression tag	UNP A9CG24
D	-2	PRO	-	expression tag	UNP A9CG24
D	-1	PHE	-	expression tag	UNP A9CG24
D	0	THR	-	expression tag	UNP A9CG24



Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP A9CG24

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Na 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	79	Total O 79 79	0	0
3	В	83	Total O 83 83	0	0
3	С	76	Total O 76 76	0	0
3	D	70	TotalO7070	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: NADQ transcription factor

SER GLY THR LYS LEU PRO LEU SER ASN

 \bullet Molecule 1: NADQ transcription factor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	58.31Å 133.34Å 86.86Å	Depositor
a, b, c, α , β , γ	90.00° 100.10° 90.00°	Depositor
Bosolution(A)	44.21 - 2.31	Depositor
	48.51 - 2.31	EDS
% Data completeness	99.7 (44.21-2.31)	Depositor
(in resolution range)	99.7 (48.51 - 2.31)	EDS
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.85 (at 2.32 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
B B.	0.199 , 0.245	Depositor
II, II, <i>free</i>	0.199 , 0.210	DCC
R_{free} test set	2788 reflections $(4.89%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	37.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ < L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9271	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: NA

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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ # Z >		RMSZ	# Z > 5
1	А	0.26	0/2331	0.54	0/3152
1	В	0.26	0/2305	0.54	0/3112
1	С	0.26	0/2246	0.53	0/3036
1	D	0.25	0/2279	0.53	0/3078
All	All	0.26	0/9161	0.54	0/12378

There are no bond length outliers.

There are no bond angle outliers.

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	А	2279	0	2229	16	0
1	В	2257	0	2227	14	0
1	С	2196	0	2152	11	0
1	D	2230	0	2178	12	0
2	D	1	0	0	0	0
3	А	79	0	0	1	0
3	В	83	0	0	0	0
3	С	76	0	0	0	0
3	D	70	0	0	0	0
All	All	9271	0	8786	47	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 3.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:57:THR:HB	1:A:104:ALA:HB2	1.74	0.69
1:D:22:PRO:HD3	1:D:239:ALA:HB1	1.83	0.60
1:A:22:PRO:HD3	1:A:239:ALA:HB1	1.82	0.60
1:A:273:ARG:NH1	1:C:55:GLU:OE1	2.35	0.59
1:A:80:LEU:HD11	1:B:3:ILE:HG21	1.87	0.56
1:A:29:GLU:HA	1:A:105:PHE:HD2	1.71	0.55
1:C:284:VAL:HA	1:C:287:GLU:HG2	1.89	0.54
1:D:230:LEU:HD23	1:D:251:ARG:HE	1.71	0.54
1:A:213:LYS:HG2	1:B:298:SER:O	2.07	0.54
1:D:246:HIS:HB3	1:D:249:ASN:HB2	1.90	0.53
1:A:53:ILE:HG21	1:A:61:VAL:HG21	1.90	0.52
1:B:238:GLU:HG2	1:B:245:LEU:HD13	1.91	0.52
1:D:122:ARG:HG3	1:D:126:LEU:HD12	1.92	0.51
1:B:230:LEU:HD23	1:B:251:ARG:HG2	1.93	0.50
1:B:251:ARG:O	1:B:255:GLU:HG2	2.12	0.50
1:A:130:ILE:O	1:A:134:ARG:HG2	2.13	0.49
1:C:150:ARG:NH2	1:C:176:GLU:OE1	2.40	0.49
1:A:209:ARG:O	1:A:213:LYS:HG3	2.14	0.48
1:C:216:TYR:O	1:C:257:GLN:NE2	2.47	0.48
1:B:249:ASN:OD1	1:B:252:ARG:NH1	2.47	0.47
1:B:157:LEU:HG	1:B:162:TRP:N	2.30	0.47
1:A:217:ARG:HG2	1:A:219:VAL:HG23	1.97	0.47
1:B:246:HIS:HB3	1:B:249:ASN:HB2	1.96	0.46
1:B:217:ARG:HG2	1:B:219:VAL:HG23	1.97	0.46
1:D:246:HIS:HE1	1:D:248:GLN:HB2	1.80	0.46
1:A:252:ARG:HG2	1:C:40:PHE:CE2	2.52	0.45
1:B:72:ASP:O	1:B:83:ARG:NH1	2.49	0.45
1:D:68:TYR:HB2	1:D:205:THR:HG21	2.00	0.44
1:A:122:ARG:HH21	1:A:130:ILE:HD12	1.83	0.44
1:D:43:ARG:HG2	1:D:44:THR:HG23	1.98	0.44
1:D:152:ASP:HB2	1:D:158:ASP:HB2	1.99	0.44
1:B:25:MET:SD	1:B:57:THR:HG21	2.59	0.43
1:D:53:ILE:HG21	1:D:61:VAL:HG21	2.00	0.42
3:A:404:HOH:O	1:B:7:HIS:HD2	2.03	0.42
1:C:29:GLU:O	1:C:193:ARG:NH2	2.53	0.41
1:D:246:HIS:CE1	1:D:248:GLN:HB2	2.55	0.41
1:C:67:LEU:HD21	1:C:90:LEU:HB2	2.03	0.41



Atom-1	Atom-2	Interatomic $distance (\hat{A})$	Clash
		distance (A)	overlap (A)
1:D:217:ARG:HG2	1:D:219:VAL:HG23	2.01	0.41
1:A:186:GLU:OE1	1:A:186:GLU:N	2.51	0.41
1:C:22:PRO:HD3	1:C:239:ALA:HB1	2.02	0.41
1:C:252:ARG:O	1:C:256:GLN:HG2	2.21	0.41
1:B:122:ARG:NH2	1:B:126:LEU:HD13	2.36	0.41
1:A:252:ARG:HA	1:A:252:ARG:HD2	1.87	0.41
1:C:290:LEU:HD13	1:D:153:PHE:HB2	2.03	0.41
1:A:257:GLN:HB2	1:A:259:LEU:HG	2.03	0.40
1:A:83:ARG:HD3	1:B:40:PHE:HA	2.03	0.40
1:C:258:GLN:HB3	1:C:281:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

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	Perce	ntiles
1	А	275/336~(82%)	265~(96%)	10 (4%)	0	100	100
1	В	264/336~(79%)	255~(97%)	9~(3%)	0	100	100
1	С	262/336~(78%)	253~(97%)	9~(3%)	0	100	100
1	D	265/336~(79%)	258~(97%)	7 (3%)	0	100	100
All	All	1066/1344~(79%)	1031 (97%)	35~(3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	F	Perce	entile	\mathbf{s}
1	А	232/278~(84%)	231 (100%)	1 (0%)		91	96	
1	В	233/278~(84%)	231~(99%)	2(1%)		78	89	
1	С	223/278~(80%)	223 (100%)	0		100	100	
1	D	226/278~(81%)	223~(99%)	3 (1%)		69	81	
All	All	914/1112 (82%)	908~(99%)	6 (1%)		84	92	

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	19	THR
1	В	294	LYS
1	В	299	ARG
1	D	142	ASP
1	D	230	LEU
1	D	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis. 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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	281/336~(83%)	0.51	14 (4%) 28 36	24, 39, 61, 111	0
1	В	276/336~(82%)	0.94	45 (16%) 1 2	25, 42, 84, 103	0
1	С	270/336~(80%)	0.68	19 (7%) 16 22	24, 38, 76, 90	0
1	D	275/336~(81%)	0.75	37 (13%) 3 4	25, 44, 75, 98	0
All	All	1102/1344 (81%)	0.72	115 (10%) 6 9	24, 41, 77, 111	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	250	PHE	6.5
1	В	231	LEU	5.7
1	В	251	ARG	5.6
1	В	248	GLN	5.2
1	D	248	GLN	5.1
1	D	161	GLY	4.9
1	А	104	ALA	4.7
1	А	186	GLU	4.6
1	В	246	HIS	4.6
1	В	299	ARG	4.4
1	В	262	GLU	4.4
1	В	298	SER	4.4
1	В	264	GLY	4.3
1	D	81	GLY	4.3
1	В	267	ALA	4.2
1	В	268	THR	4.2
1	А	68	TYR	4.0
1	С	254	ILE	4.0
1	В	75	ARG	3.9
1	В	263	THR	3.8
1	В	158	ASP	3.8



7Q91

Mol	Chain	Res	Type	RSRZ
1	D	141	PRO	3.7
1	D	142	ASP	3.7
1	D	139	SER	3.6
1	В	266	MET	3.6
1	А	188	ARG	3.4
1	В	252	ARG	3.4
1	В	216	TYR	3.3
1	В	276	LYS	3.3
1	D	291	SER	3.2
1	В	300	ASN	3.2
1	D	76	ASN	3.1
1	А	159	GLY	3.1
1	D	264	GLY	3.0
1	D	273	ARG	3.0
1	A	157	LEU	2.9
1	D	189	ILE	2.9
1	В	279	ARG	2.9
1	А	142	ASP	2.9
1	D	252	ARG	2.9
1	В	227	SER	2.8
1	В	156	GLY	2.8
1	В	247	LYS	2.8
1	С	80	LEU	2.8
1	D	279	ARG	2.8
1	А	291	SER	2.8
1	В	297	LEU	2.8
1	С	81	GLY	2.8
1	А	105	PHE	2.8
1	В	249	ASN	2.8
1	D	256	GLN	2.8
1	В	258	GLN	2.7
1	В	124	ASP	2.7
1	D	251	ARG	2.7
1	В	1	VAL	2.7
1	D	247	LYS	2.7
1	В	256	GLN	2.6
1	D	145	ALA	2.6
1	С	275	ALA	2.6
1	В	20	ASP	2.6
1	С	96	GLN	2.6
1	С	249	ASN	2.6
1	D	40	PHE	2.6



7Q91

Mol	Chain	Res	Type	RSRZ	
1	D	138	ASP	2.5	
1	D	127	ASP	2.5	
1	С	266	MET	2.5	
1	С	248	GLN	2.5	
1	D	134	ARG	2.5	
1	D	146	GLN	2.5	
1	D	260	VAL	2.5	
1	В	187	PRO	2.5	
1	С	256	GLN	2.5	
1	В	254	ILE	2.4	
1	С	285	LEU	2.4	
1	D	258	GLN	2.4	
1	D	277	LEU	2.4	
1	D	153	PHE	2.4	
1	D	158	ASP	2.4	
1	В	208	ALA	2.4	
1	В	255	GLU	2.4	
1	В	278	PHE	2.4	
1	А	185	SER	2.3	
1	С	262	GLU	2.3	
1	С	258	GLN	2.3	
1	В	131	ASP	2.3	
1	А	67	LEU	2.3	
1	D	148	HIS	2.3	
1	D	255	GLU	2.3	
1	D	270	THR	2.2	
1	В	82	GLY	2.2	
1	В	196	PHE	2.2	
1	D	124	ASP	2.2	
1	D	143	SER	2.2	
1	В	106	TRP	2.2	
1	D	254	ILE	2.2	
1	С	283	THR	2.2	
1	D	263	THR	2.2	
1	А	79	ILE	2.2	
1	В	261	GLU	2.2	
1	В	230	LEU	2.1	
1	В	277	LEU	2.1	
1	С	94	ARG	2.1	
1	А	52	TRP	2.1	
1	С	146	GLN	2.1	
1	D	261	GLU	2.1	



		1	1 5	
Mol	Chain	Res	Type	RSRZ
1	D	226	ASP	2.1
1	С	290	LEU	2.1
1	А	270	THR	2.1
1	В	67	LEU	2.1
1	С	216	TYR	2.1
1	В	226	ASP	2.0
1	В	233	LEU	2.0
1	С	255	GLU	2.0
1	С	280	PHE	2.0
1	D	249	ASN	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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	NA	D	401	1/1	0.95	0.24	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.

