



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:32 PM EDT

PDB ID : 7FM9 / pdb_00007fm9
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P06B02 from the F2X-Universal Library
Authors : Barthel, T.; Wollenhaupt, J.; Lima, G.M.A.; Wahl, M.C.; Weiss, M.S.
Deposited on : 2022-08-26
Resolution : 1.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

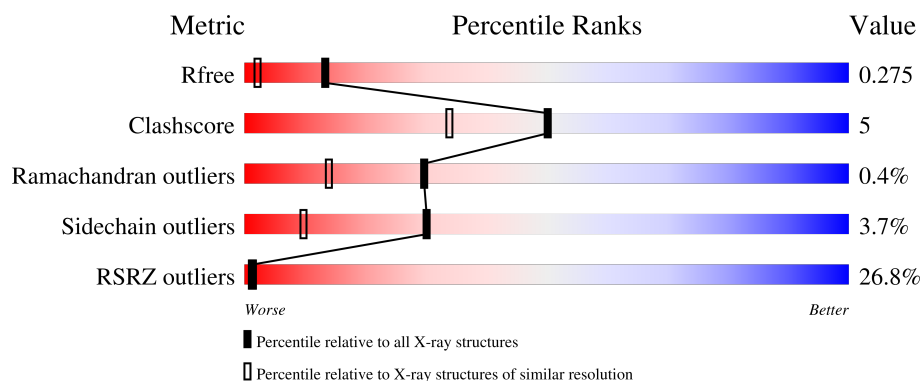
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	258	
2	B	308	

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
3	VQQ	B	401	-	X	-	-
3	VQQ	B	404	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9221 atoms, of which 4518 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	237	4068	1287	2060	336	373	12	18	21	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	300	5033	1651	2458	420	484	20	0	16	0

There are 20 discrepancies between the modelled and reference sequences:

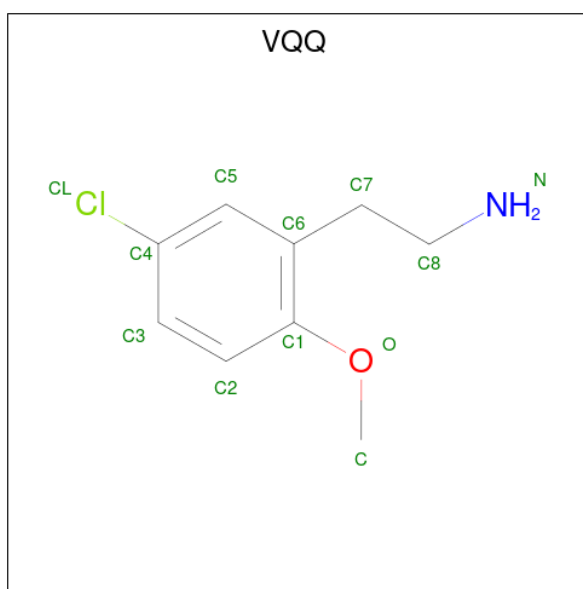
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	SER	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	170	SER	ASP	conflict	UNP P32357

- Molecule 3 is 2-(5-chloro-2-methoxyphenyl)ethan-1-amine (CCD ID: VQQ) (formula: $C_9H_{12}ClNO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			12	9	1	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			12	9	1	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			12	9	1	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			12	9	1	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		

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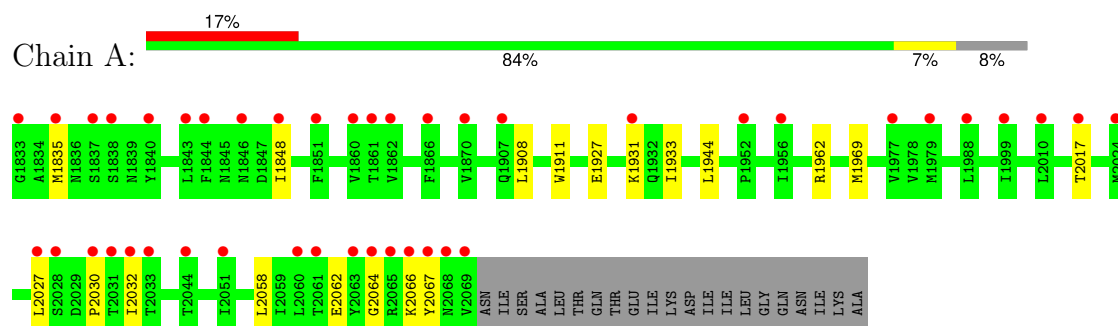
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	29	Total	O	0	0
			29	29		

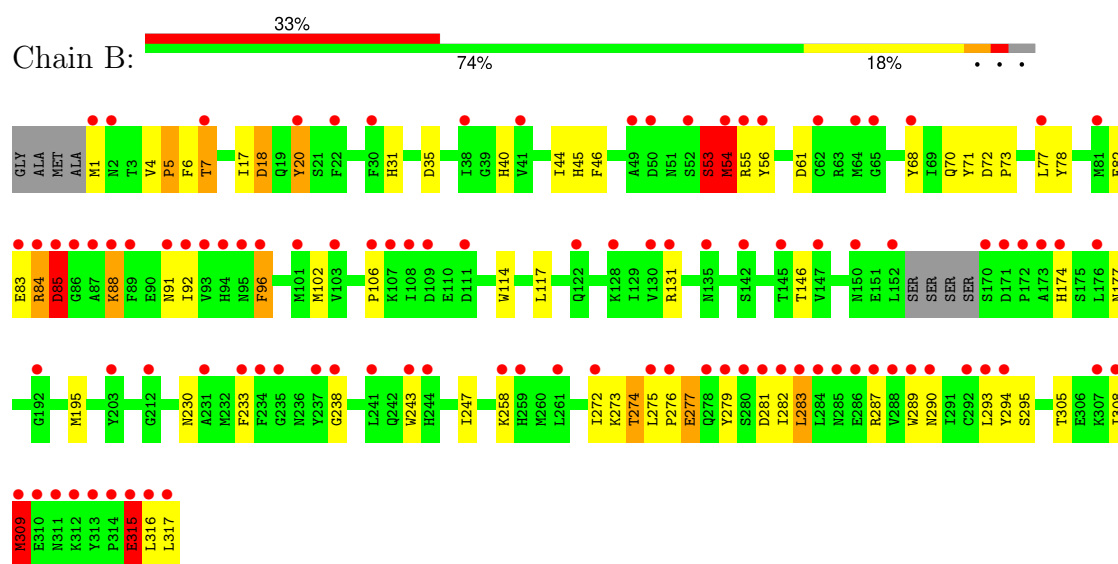
3 Residue-property plots

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: Pre-mRNA-splicing factor 8



• Molecule 2: A1 cistron-splicing factor AAR2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.02Å 81.66Å 94.43Å 90.00° 109.07° 90.00°	Depositor
Resolution (Å)	40.83 – 1.59 40.83 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.83-1.59) 99.7 (40.83-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.220 , 0.259 0.261 , 0.275	Depositor DCC
R_{free} test set	2095 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.69	3/2149 (0.1%)	0.75	2/2911 (0.1%)
2	B	0.97	15/2731 (0.5%)	1.25	40/3688 (1.1%)
All	All	0.86	18/4880 (0.4%)	1.05	42/6599 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	PRO	N-CA	14.27	1.64	1.47
1	A	2030	PRO	C-O	-9.06	1.12	1.24
1	A	2064	GLY	C-O	-7.99	1.14	1.23
2	B	233	PHE	C-O	-7.81	1.14	1.24
2	B	230	ASN	C-O	7.20	1.32	1.24
2	B	4	VAL	C-N	7.10	1.42	1.33
2	B	44[A]	ILE	C-N	6.95	1.43	1.33
2	B	44[B]	ILE	C-N	6.95	1.43	1.33
2	B	20	TYR	C-O	-6.89	1.15	1.23
2	B	18	ASP	CG-OD2	-6.88	1.12	1.25
2	B	71	TYR	C-O	-6.85	1.15	1.23
2	B	18	ASP	C-O	-6.70	1.17	1.24
2	B	70	GLN	C-O	-6.56	1.16	1.24
2	B	78	TYR	C-O	-6.38	1.16	1.24
2	B	72	ASP	C-O	-5.94	1.17	1.24
1	A	2032	ILE	C-N	5.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	ASP	CG-OD2	-5.19	1.15	1.25
2	B	73	PRO	C-O	-5.05	1.18	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	VAL	CA-C-N	16.01	136.02	119.85
2	B	4	VAL	C-N-CA	16.01	136.02	119.85
2	B	5	PRO	CB-CA-C	11.45	125.98	110.98
2	B	230	ASN	CA-C-O	9.82	130.96	120.55
1	A	2027	LEU	O-C-N	-8.84	112.60	122.23
2	B	315	GLU	CA-C-N	8.11	131.14	120.28
2	B	315	GLU	C-N-CA	8.11	131.14	120.28
1	A	2032	ILE	CA-C-O	-8.02	111.53	120.84
2	B	7	THR	N-CA-C	-7.91	102.26	112.23
2	B	7	THR	CA-CB-OG1	-7.84	97.85	109.60
2	B	5	PRO	N-CA-C	-7.74	99.08	111.38
2	B	5	PRO	CA-N-CD	-7.66	101.28	112.00
2	B	230	ASN	N-CA-C	7.38	119.32	111.28
2	B	7	THR	CA-C-O	-7.21	111.28	119.79
2	B	45[A]	HIS	CA-CB-CG	6.60	120.40	113.80
2	B	45[B]	HIS	CA-CB-CG	6.60	120.40	113.80
2	B	276	PRO	CA-C-N	6.31	129.03	120.38
2	B	276	PRO	C-N-CA	6.31	129.03	120.38
2	B	88	LYS	N-CA-C	-6.22	104.50	111.28
2	B	44[A]	ILE	CA-C-N	-5.91	112.88	122.81
2	B	44[A]	ILE	C-N-CA	-5.91	112.88	122.81
2	B	44[B]	ILE	CA-C-N	-5.91	112.88	122.81
2	B	44[B]	ILE	C-N-CA	-5.91	112.88	122.81
2	B	96	PHE	CA-CB-CG	5.90	119.70	113.80
2	B	230	ASN	O-C-N	-5.86	115.91	122.12
2	B	91	ASN	CA-C-N	5.82	128.00	120.56
2	B	91	ASN	C-N-CA	5.82	128.00	120.56
2	B	53	SER	CA-C-O	-5.64	114.32	120.81
2	B	277	GLU	CA-C-N	5.61	129.58	120.60
2	B	277	GLU	C-N-CA	5.61	129.58	120.60
2	B	44[A]	ILE	O-C-N	5.59	129.23	123.03
2	B	44[B]	ILE	O-C-N	5.59	129.23	123.03
2	B	309	MET	CA-C-O	-5.36	115.19	120.82
2	B	277	GLU	CB-CG-CD	5.35	121.69	112.60
2	B	6	PHE	CA-CB-CG	5.31	119.11	113.80
2	B	293	LEU	O-C-N	5.26	128.54	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ILE	CA-C-N	5.26	129.62	120.68
2	B	272	ILE	C-N-CA	5.26	129.62	120.68
2	B	233	PHE	CA-C-O	-5.21	113.64	119.79
2	B	274	THR	N-CA-C	-5.14	105.36	111.69
2	B	5	PRO	N-CD-CG	5.03	110.74	103.20
2	B	7	THR	O-C-N	5.03	129.07	122.33

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	53	SER	Mainchain
2	B	54[A]	MET	Mainchain
2	B	54[B]	MET	Mainchain

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	2008	2060	1974	11	1
2	B	2575	2458	2392	39	1
3	B	48	0	0	2	0
4	A	43	0	0	1	0
4	B	29	0	0	2	0
All	All	4703	4518	4366	48	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (48) 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)
2:B:283:LEU:O	2:B:283:LEU:HD22	1.78	0.83
2:B:117:LEU:HD11	2:B:274:THR:HG21	1.61	0.82
2:B:85:ASP:OD1	2:B:88:LYS:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:GLU:O	4:B:501:HOH:O	2.08	0.70
2:B:85:ASP:O	2:B:88:LYS:N	2.28	0.65
1:A:1927:GLU:OE1	4:A:2101:HOH:O	2.16	0.62
2:B:243:TRP:NE1	2:B:247:ILE:HD11	2.13	0.62
2:B:83:GLU:OE2	2:B:88:LYS:HD3	2.00	0.61
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ3	1.51	0.58
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.30	0.57
2:B:20:TYR:CD2	2:B:106:PRO:HD2	2.40	0.56
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.89	0.54
1:A:1911:TRP:CD1	2:B:195:MET:HE3	2.42	0.54
1:A:2017[B]:THR:HG22	1:A:2062:GLU:HG2	1.90	0.54
2:B:83:GLU:HA	2:B:83:GLU:OE1	2.08	0.53
2:B:83:GLU:OE2	2:B:88:LYS:CD	2.59	0.51
2:B:84:ARG:CZ	2:B:84:ARG:CB	2.90	0.49
2:B:7:THR:HG22	3:B:401:VQQ:C4	2.43	0.49
2:B:84:ARG:NH1	2:B:84:ARG:HB3	2.27	0.48
1:A:1969:MET:HA	1:A:1969:MET:HE2	1.95	0.48
2:B:315:GLU:CD	2:B:315:GLU:N	2.72	0.48
2:B:84:ARG:CZ	2:B:84:ARG:HB3	2.43	0.47
2:B:281:ASP:N	2:B:281:ASP:OD1	2.47	0.47
2:B:40:HIS:HD2	4:B:507:HOH:O	1.97	0.47
2:B:294:TYR:CE2	2:B:317:LEU:HD13	2.50	0.46
2:B:18:ASP:HB3	2:B:114:TRP:CE3	2.51	0.46
2:B:283:LEU:HD22	2:B:283:LEU:C	2.38	0.46
1:A:2067:TYR:CD1	1:A:2067:TYR:N	2.84	0.45
2:B:46:PHE:HB2	2:B:56:TYR:CZ	2.52	0.45
2:B:305:THR:O	2:B:309:MET:HG3	2.18	0.44
2:B:287:ARG:O	2:B:287:ARG:HG2	2.16	0.44
1:A:1908:LEU:HA	2:B:195:MET:HE1	1.99	0.43
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.83	0.43
2:B:68:TYR:OH	3:B:401:VQQ:N	2.51	0.43
2:B:54[A]:MET:HE3	2:B:56:TYR:CD1	2.54	0.43
2:B:258:LYS:HD2	2:B:258:LYS:H	1.84	0.43
2:B:77:LEU:N	2:B:77:LEU:HD23	2.35	0.42
2:B:5:PRO:HA	2:B:31:HIS:O	2.20	0.42
2:B:20:TYR:CE2	2:B:106:PRO:HD2	2.55	0.42
1:A:1933:ILE:HG21	1:A:1944:LEU:HD21	2.01	0.42
2:B:243:TRP:CZ2	2:B:289:TRP:HZ2	2.38	0.41
2:B:146:THR:HG23	2:B:238:GLY:HA3	2.02	0.41
2:B:131:ARG:HH21	2:B:177[B]:ASN:ND2	2.19	0.41
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LYS:H	2:B:258:LYS:CD	2.34	0.41
2:B:1:MET:HB3	2:B:35:ASP:HA	2.04	0.40
2:B:54[A]:MET:HE2	2:B:54[A]:MET:HB3	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2066:LYS:HG2	2:B:279:TYR:HE1[2_655]	1.27	0.33

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/258 (100%)	252 (98%)	6 (2%)	0	100	100
2	B	314/308 (102%)	299 (95%)	12 (4%)	3 (1%)	12	3
All	All	572/566 (101%)	551 (96%)	18 (3%)	3 (0%)	30	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54[A]	MET
2	B	54[B]	MET
2	B	85	ASP

5.3.2 Protein sidechains [i](#)

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	237/233 (102%)	237 (100%)	0	100	100
2	B	293/284 (103%)	274 (94%)	19 (6%)	15	3
All	All	530/517 (102%)	511 (96%)	19 (4%)	30	10

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	17	ILE
2	B	53	SER
2	B	55[A]	ARG
2	B	55[B]	ARG
2	B	82	GLU
2	B	84	ARG
2	B	85	ASP
2	B	92	ILE
2	B	174	HIS
2	B	273	LYS
2	B	275	LEU
2	B	282	ILE
2	B	283	LEU
2	B	290	ASN
2	B	295	SER
2	B	308	ILE
2	B	309	MET
2	B	315	GLU
2	B	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	259	HIS
2	B	290	ASN

5.3.3 RNA ⓘ

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
3	VQQ	B	401	-	12,12,12	3.48	9 (75%)	15,15,15	2.97	11 (73%)
3	VQQ	B	402	-	12,12,12	2.56	5 (41%)	15,15,15	1.45	3 (20%)
3	VQQ	B	403	-	12,12,12	1.91	3 (25%)	15,15,15	1.40	2 (13%)
3	VQQ	B	404	-	12,12,12	5.31	8 (66%)	15,15,15	4.57	13 (86%)

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
3	VQQ	B	401	-	-	2/5/5/5	0/1/1/1
3	VQQ	B	402	-	-	2/5/5/5	0/1/1/1
3	VQQ	B	403	-	-	1/5/5/5	0/1/1/1
3	VQQ	B	404	-	-	4/5/5/5	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	VQQ	C4-CL	-9.78	1.51	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	VQQ	C7-C6	-8.53	1.35	1.51
3	B	404	VQQ	C2-C3	-8.43	1.25	1.38
3	B	404	VQQ	C3-C4	-7.61	1.24	1.38
3	B	401	VQQ	C5-C6	-6.76	1.28	1.39
3	B	402	VQQ	C4-CL	-6.39	1.59	1.74
3	B	401	VQQ	C5-C4	-4.82	1.30	1.38
3	B	403	VQQ	C4-CL	-4.14	1.64	1.74
3	B	401	VQQ	C7-C6	-4.09	1.44	1.51
3	B	404	VQQ	C2-C1	-4.06	1.31	1.39
3	B	401	VQQ	C2-C3	-3.82	1.32	1.38
3	B	403	VQQ	O-C1	-3.66	1.31	1.37
3	B	401	VQQ	O-C1	-3.48	1.31	1.37
3	B	401	VQQ	C3-C4	-3.25	1.32	1.38
3	B	402	VQQ	C2-C3	-3.00	1.34	1.38
3	B	404	VQQ	O-C1	-2.84	1.32	1.37
3	B	401	VQQ	O-C	-2.80	1.35	1.42
3	B	402	VQQ	C1-C6	-2.76	1.35	1.39
3	B	401	VQQ	C8-C7	-2.62	1.42	1.51
3	B	404	VQQ	C5-C4	-2.59	1.34	1.38
3	B	402	VQQ	O-C1	-2.50	1.33	1.37
3	B	401	VQQ	C4-CL	2.33	1.79	1.74
3	B	404	VQQ	O-C	-2.11	1.36	1.42
3	B	403	VQQ	C7-C6	-2.05	1.47	1.51
3	B	402	VQQ	C7-C6	-2.02	1.47	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	VQQ	O-C1-C6	9.02	129.38	115.96
3	B	404	VQQ	C3-C4-CL	-8.10	107.40	119.36
3	B	404	VQQ	C5-C4-CL	6.49	127.31	119.17
3	B	404	VQQ	O-C1-C2	-5.57	114.90	124.30
3	B	401	VQQ	C3-C4-CL	4.78	126.41	119.36
3	B	404	VQQ	C7-C6-C1	4.20	128.40	121.29
3	B	401	VQQ	C7-C6-C1	4.10	128.24	121.29
3	B	401	VQQ	C7-C8-N	-4.10	101.47	112.71
3	B	401	VQQ	C7-C6-C5	-3.89	111.70	119.38
3	B	403	VQQ	C8-C7-C6	-3.69	105.08	112.85
3	B	404	VQQ	C7-C8-N	-3.66	102.69	112.71
3	B	404	VQQ	C4-C5-C6	-3.54	115.31	119.96
3	B	404	VQQ	C7-C6-C5	-3.49	112.50	119.38
3	B	401	VQQ	C2-C3-C4	3.24	122.50	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	VQQ	C-O-C1	-3.12	112.93	117.51
3	B	401	VQQ	C4-C5-C6	3.04	123.97	119.96
3	B	402	VQQ	C8-C7-C6	-3.02	106.48	112.85
3	B	401	VQQ	C3-C4-C5	-2.97	117.65	121.53
3	B	401	VQQ	C5-C4-CL	-2.91	115.52	119.17
3	B	404	VQQ	C8-C7-C6	-2.76	107.03	112.85
3	B	404	VQQ	C2-C1-C6	-2.59	115.69	120.18
3	B	401	VQQ	C-O-C1	2.58	121.30	117.51
3	B	401	VQQ	C2-C1-C6	-2.47	115.90	120.18
3	B	404	VQQ	C3-C2-C1	2.45	124.71	120.06
3	B	404	VQQ	C3-C4-C5	2.34	124.60	121.53
3	B	402	VQQ	C3-C4-CL	-2.20	116.11	119.36
3	B	401	VQQ	C8-C7-C6	-2.18	108.25	112.85
3	B	403	VQQ	C-O-C1	-2.02	114.55	117.51
3	B	402	VQQ	C4-C5-C6	-2.02	117.31	119.96

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	VQQ	C6-C7-C8-N
3	B	402	VQQ	C1-C6-C7-C8
3	B	403	VQQ	C1-C6-C7-C8
3	B	404	VQQ	C1-C6-C7-C8
3	B	404	VQQ	C5-C6-C7-C8
3	B	404	VQQ	C2-C1-O-C
3	B	404	VQQ	C6-C1-O-C
3	B	401	VQQ	C5-C6-C7-C8
3	B	401	VQQ	C1-C6-C7-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	VQQ	2	0

5.7 Other polymers [i](#)

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, 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	237/258 (91%)	1.33	43 (18%) 3 3	18, 54, 86, 107	12 (5%)
2	B	300/308 (97%)	1.89	101 (33%) 1 1	18, 60, 98, 127	8 (2%)
All	All	537/566 (94%)	1.64	144 (26%) 1 1	18, 57, 93, 127	20 (3%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	288	VAL	9.0
2	B	289	TRP	8.2
2	B	316	LEU	8.1
2	B	152	LEU	7.9
2	B	317	LEU	7.5
1	A	2069	VAL	7.0
2	B	170	SER	7.0
2	B	85	ASP	7.0
2	B	282	ILE	6.7
2	B	272	ILE	5.9
2	B	243	TRP	5.8
2	B	313	TYR	5.8
2	B	54[A]	MET	5.7
2	B	283	LEU	5.2
2	B	279	TYR	4.9
2	B	203[A]	TYR	4.9
1	A	2066	LYS	4.9
2	B	108	ILE	4.8
1	A	2032	ILE	4.8
2	B	314	PRO	4.7
2	B	311	ASN	4.6
1	A	2063	TYR	4.6
2	B	101	MET	4.6
1	A	1979[A]	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	2065	ARG	4.3
2	B	172	PRO	4.2
2	B	294	TYR	4.2
2	B	275	LEU	4.2
1	A	2051	ILE	4.1
1	A	1866	PHE	4.0
2	B	309	MET	4.0
2	B	307	LYS	4.0
2	B	276	PRO	4.0
2	B	84	ARG	4.0
2	B	86	GLY	3.9
1	A	2061	THR	3.9
2	B	122[A]	GLN	3.7
2	B	237	TYR	3.7
1	A	1860	VAL	3.6
2	B	174	HIS	3.6
1	A	1833	GLY	3.6
1	A	2031	THR	3.5
1	A	1840	TYR	3.5
2	B	49	ALA	3.5
2	B	173	ALA	3.5
2	B	41[A]	VAL	3.5
2	B	290	ASN	3.4
2	B	308	ILE	3.4
2	B	285	ASN	3.4
1	A	2067	TYR	3.4
2	B	1	MET	3.3
2	B	89	PHE	3.3
2	B	96	PHE	3.3
1	A	2030	PRO	3.3
2	B	293	LEU	3.3
2	B	92	ILE	3.3
2	B	315	GLU	3.2
2	B	68	TYR	3.2
2	B	278	GLN	3.2
2	B	238	GLY	3.2
2	B	55[A]	ARG	3.1
2	B	234	PHE	3.1
2	B	231	ALA	3.1
1	A	1835	MET	3.1
1	A	2017[A]	THR	3.1
2	B	286	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1931[A]	LYS	3.1
1	A	1861	THR	3.0
1	A	2068	ASN	3.0
2	B	147	VAL	3.0
2	B	287	ARG	3.0
1	A	2028	SER	3.0
2	B	235	GLY	2.9
2	B	244	HIS	2.9
1	A	1988	LEU	2.9
2	B	312	LYS	2.9
1	A	2060	LEU	2.9
2	B	284	LEU	2.9
2	B	22	PHE	2.9
1	A	2064	GLY	2.9
2	B	56	TYR	2.8
2	B	281	ASP	2.8
2	B	131	ARG	2.8
1	A	1870	VAL	2.7
2	B	83	GLU	2.7
2	B	241	LEU	2.7
2	B	62	CYS	2.7
2	B	95	ASN	2.6
1	A	1907	GLN	2.6
1	A	1999	ILE	2.6
1	A	2010	LEU	2.6
2	B	52	SER	2.6
2	B	38	ILE	2.6
2	B	30	PHE	2.6
2	B	2	ASN	2.6
2	B	258	LYS	2.5
1	A	1977	VAL	2.5
1	A	1844	PHE	2.5
1	A	1862	VAL	2.5
2	B	103	VAL	2.5
2	B	88	LYS	2.5
1	A	2044	THR	2.5
2	B	93	VAL	2.5
1	A	2033	THR	2.4
1	A	1848	ILE	2.4
2	B	91	ASN	2.4
1	A	1843	LEU	2.4
2	B	7	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1851	PHE	2.4
2	B	81	MET	2.3
2	B	145	THR	2.3
2	B	130	VAL	2.3
2	B	142	SER	2.3
2	B	20	TYR	2.3
2	B	107	LYS	2.3
2	B	150	ASN	2.3
2	B	64[A]	MET	2.3
1	A	1838	SER	2.3
2	B	109	ASP	2.2
2	B	50	ASP	2.2
1	A	1956	ILE	2.2
1	A	1846	ASN	2.2
1	A	2024[A]	MET	2.2
2	B	94	HIS	2.2
2	B	176	LEU	2.1
2	B	259	HIS	2.1
2	B	65[A]	GLY	2.1
2	B	87	ALA	2.1
2	B	106	PRO	2.1
2	B	261	LEU	2.1
2	B	212[A]	GLY	2.1
2	B	310	GLU	2.1
1	A	1952	PRO	2.1
2	B	77	LEU	2.1
2	B	292	CYS	2.1
2	B	111	ASP	2.1
2	B	192	GLY	2.1
2	B	233	PHE	2.0
1	A	2027	LEU	2.0
2	B	280	SER	2.0
2	B	135	ASN	2.0
2	B	128	LYS	2.0
1	A	1837	SER	2.0
2	B	171	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VQQ	B	403	12/12	0.73	0.24	20,20,20,20	12
3	VQQ	B	401	12/12	0.78	0.20	20,20,20,20	12
3	VQQ	B	404	12/12	0.78	0.21	20,20,20,20	12
3	VQQ	B	402	12/12	0.79	0.22	20,20,20,20	12

6.5 Other polymers [i](#)

There are no such residues in this entry.