



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 07:52 PM EDT

PDB ID : 5SU7  
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P03E12 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 : 1.81 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

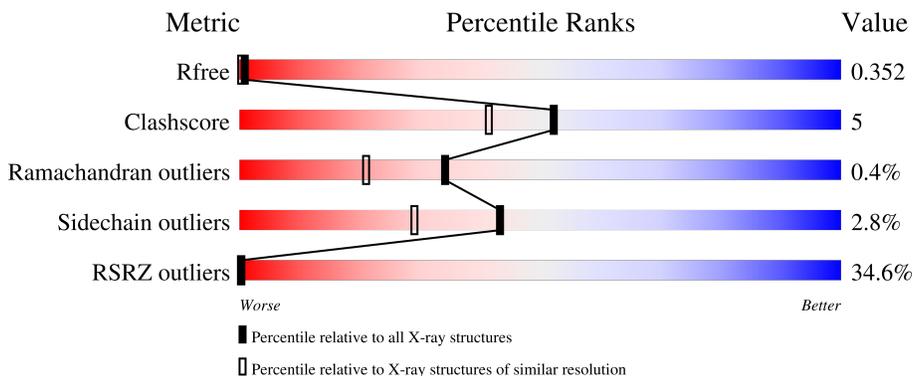
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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))
$R_{free}$	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9164 atoms, of which 4524 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	0	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	5044	1654	2464	421	485	20	11	17	0

There are 20 discrepancies between the modelled and reference sequences:

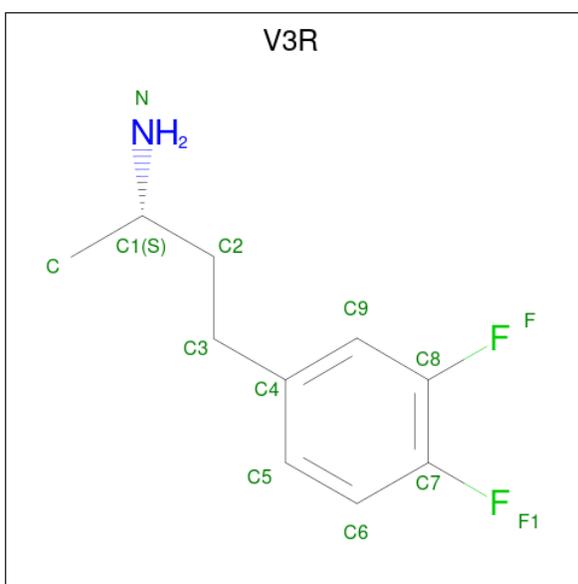
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 (2S)-4-(3,4-difluorophenyl)butan-2-amine (three-letter code: V3R) (formula: C<sub>10</sub>H<sub>13</sub>F<sub>2</sub>N).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
3	B	1	13	10	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	16	Total	O	0	0
			16	16		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.39Å 81.82Å 93.72Å 90.00° 108.03° 90.00°	Depositor
Resolution (Å)	44.75 – 1.81 44.74 – 1.81	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.75-1.81) 97.9 (44.74-1.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 1.81Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.318 , 0.346 0.326 , 0.352	Depositor DCC
$R_{free}$ test set	2100 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtrriage
Anisotropy	0.322	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9164	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: V3R

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	0.78	3/2149 (0.1%)	0.82	0/2911
2	B	0.88	6/2739 (0.2%)	0.89	5/3699 (0.1%)
All	All	0.84	9/4888 (0.2%)	0.86	5/6610 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1878	CYS	CB-SG	-7.29	1.69	1.82
1	A	1879	ILE	CB-CG2	6.60	1.73	1.52
1	A	1851	PHE	CG-CD2	6.50	1.48	1.38
2	B	292	CYS	CB-SG	-6.13	1.71	1.82
2	B	105	TYR	CG-CD2	5.95	1.46	1.39
2	B	114	TRP	CG-CD1	-5.91	1.28	1.36
2	B	105	TYR	CG-CD1	-5.64	1.31	1.39
2	B	239	SER	CB-OG	-5.62	1.34	1.42
2	B	114	TRP	CE2-CZ2	5.15	1.48	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	PHE	CB-CG-CD2	-6.69	116.12	120.80
2	B	7	THR	CA-C-O	-5.59	108.36	120.10
2	B	117	LEU	CB-CG-CD1	-5.45	101.73	111.00
2	B	72	ASP	CB-CG-OD1	5.31	123.08	118.30
2	B	18	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2008	2060	1974	15	0
2	B	2580	2464	2396	35	0
3	B	13	0	0	1	0
4	A	23	0	0	0	0
4	B	16	0	0	0	0
All	All	4640	4524	4370	50	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 (50) 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:88:LYS:HD3	2:B:92:ILE:HD11	1.18	1.09
2:B:88:LYS:CD	2:B:92:ILE:HD11	1.99	0.92
2:B:287:ARG:O	2:B:291:ILE:HD13	1.79	0.83
2:B:88:LYS:HD3	2:B:92:ILE:CD1	2.07	0.81
2:B:4:VAL:HG11	2:B:44[B]:ILE:CD1	2.19	0.72
1:A:2061:THR:O	1:A:2064:GLY:N	2.21	0.71
2:B:4:VAL:HG11	2:B:44[B]:ILE:HD12	1.72	0.71
2:B:80:MET:HG2	2:B:137:PHE:CE2	2.29	0.68
2:B:88:LYS:O	2:B:92:ILE:HG12	1.97	0.65
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.33	0.62
2:B:80:MET:HG2	2:B:137:PHE:CD2	2.35	0.62
2:B:4:VAL:HG23	2:B:36:ILE:CD1	2.30	0.61
2:B:80:MET:HG2	2:B:137:PHE:CZ	2.41	0.56
2:B:1:MET:HB3	2:B:35:ASP:HA	1.87	0.55
2:B:4:VAL:HG23	2:B:36:ILE:HD12	1.90	0.54
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.73	0.53
2:B:258:LYS:HD2	2:B:258:LYS:H	1.73	0.53
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.44	0.53
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.91	0.53
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.93	0.50
2:B:80:MET:HG2	2:B:137:PHE:CG	2.46	0.50
1:A:1910:LYS:O	1:A:1940:MET:HE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.48	0.49
2:B:110:GLU:HG2	2:B:110:GLU:O	2.16	0.46
2:B:68:TYR:OH	3:B:401:V3R:C	2.63	0.46
2:B:2:ASN:HB3	2:B:62:CYS:SG	2.56	0.46
1:A:2064:GLY:O	1:A:2068:ASN:N	2.48	0.46
1:A:2062:GLU:O	1:A:2066:LYS:HB2	2.15	0.46
2:B:8:SER:C	2:B:10:PRO:HD3	2.36	0.45
2:B:80:MET:SD	2:B:137:PHE:CG	3.10	0.45
2:B:277:GLU:CD	2:B:277:GLU:H	2.20	0.45
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	1.99	0.44
2:B:56:TYR:CE2	2:B:77:LEU:HB2	2.53	0.44
1:A:2044:THR:OG1	1:A:2047:GLN:HG3	2.17	0.44
2:B:43:VAL:HG13	2:B:43:VAL:O	2.19	0.42
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.34	0.42
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.19	0.42
2:B:77:LEU:N	2:B:77:LEU:HD23	2.34	0.41
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	2.02	0.41
2:B:44[A]:ILE:HG23	2:B:44[A]:ILE:O	2.21	0.41
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.33	0.41
1:A:1882:LEU:HD12	1:A:1888:HIS:O	2.21	0.41
2:B:1:MET:N	2:B:38:ILE:HD11	2.36	0.41
2:B:80:MET:HG2	2:B:137:PHE:CE1	2.56	0.40
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.57	0.40
2:B:1:MET:H2	2:B:38:ILE:HD11	1.85	0.40
2:B:131:ARG:HH21	2:B:177[B]:ASN:ND2	2.19	0.40
1:A:1835:MET:H	1:A:1959:THR:HA	1.87	0.40
2:B:80:MET:HG2	2:B:137:PHE:CD1	2.57	0.40
2:B:275:LEU:HD21	2:B:283:LEU:HD13	2.02	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	Percentiles	
1	A	258/258 (100%)	243 (94%)	14 (5%)	1 (0%)	34	21
2	B	315/308 (102%)	299 (95%)	14 (4%)	2 (1%)	25	12
All	All	573/566 (101%)	542 (95%)	28 (5%)	3 (0%)	34	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2068	ASN
2	B	54[A]	MET
2	B	54[B]	MET

### 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%)	229 (97%)	8 (3%)	37	22
2	B	294/284 (104%)	286 (97%)	8 (3%)	44	30
All	All	531/517 (103%)	515 (97%)	16 (3%)	43	26

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1962	ARG
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
1	A	2020	GLU
1	A	2060	LEU
1	A	2066	LYS
2	B	2	ASN
2	B	80	MET
2	B	84	ARG
2	B	92	ILE
2	B	258	LYS

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Mol	Chain	Res	Type
2	B	275	LEU
2	B	281	ASP
2	B	295	SER

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

Mol	Chain	Res	Type
1	A	1947	HIS
2	B	47	GLN
2	B	70	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	V3R	B	401	-	13,13,13	1.30	3 (23%)	16,17,17	1.04	1 (6%)

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	V3R	B	401	-	-	5/5/5/5	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	V3R	C1-N	2.67	1.56	1.49
3	B	401	V3R	F1-C7	-2.27	1.29	1.35
3	B	401	V3R	F-C8	-2.11	1.30	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	V3R	C4-C9-C8	-2.83	117.53	119.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	V3R	C1-C2-C3-C4
3	B	401	V3R	N-C1-C2-C3
3	B	401	V3R	C-C1-C2-C3
3	B	401	V3R	C2-C3-C4-C9
3	B	401	V3R	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	V3R	1	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 [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<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	237/258 (91%)	1.90	81 (34%) 0 0	46, 90, 179, 254	0
2	B	300/308 (97%)	1.90	105 (35%) 0 0	49, 88, 188, 276	0
All	All	537/566 (94%)	1.90	186 (34%) 0 0	46, 89, 182, 276	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2068	ASN	19.5
1	A	1833	GLY	19.1
2	B	52	SER	10.9
2	B	53	SER	9.8
2	B	1	MET	9.6
2	B	171	ASP	9.5
1	A	2069	VAL	9.3
2	B	151	GLU	9.0
1	A	2027	LEU	8.4
2	B	133	ASP	8.3
1	A	2028	SER	7.8
1	A	2032	ILE	6.8
1	A	2067	TYR	6.6
1	A	2039	LEU	6.6
1	A	2064	GLY	6.4
1	A	1838	SER	6.4
2	B	172	PRO	6.1
2	B	109	ASP	6.0
2	B	107	LYS	5.9
1	A	2040	TRP	5.8
1	A	2063	TYR	5.7
1	A	2065	ARG	5.7
2	B	316	LEU	5.5
2	B	54[A]	MET	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	277	GLU	5.3
2	B	124	ASP	5.2
2	B	62	CYS	5.1
1	A	1836	ASN	5.1
1	A	1834	ALA	5.0
2	B	279	TYR	5.0
1	A	2060	LEU	4.7
2	B	101	MET	4.7
2	B	20	TYR	4.7
1	A	1866	PHE	4.6
2	B	170	SER	4.6
1	A	2066	LYS	4.5
2	B	108	ILE	4.5
1	A	2044	THR	4.5
2	B	150	ASN	4.4
2	B	131	ARG	4.4
2	B	283	LEU	4.3
2	B	38	ILE	4.2
2	B	102	MET	4.1
1	A	1964	PRO	4.0
2	B	84	ARG	4.0
2	B	313	TYR	4.0
1	A	2048	TRP	4.0
2	B	276	PRO	3.9
1	A	2046	GLU	3.9
2	B	103	VAL	3.8
2	B	203[A]	TYR	3.8
2	B	74	LYS	3.8
2	B	122[A]	GLN	3.8
2	B	110	GLU	3.8
1	A	2053[A]	SER	3.8
2	B	80	MET	3.7
2	B	295	SER	3.7
2	B	93	VAL	3.7
2	B	15	ILE	3.7
2	B	280	SER	3.7
2	B	19	GLN	3.7
2	B	291	ILE	3.6
2	B	293	LEU	3.6
2	B	148	GLN	3.6
2	B	17	ILE	3.6
1	A	2024[A]	MET	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1963	LEU	3.5
1	A	1875	ILE	3.5
2	B	147	VAL	3.5
2	B	195	MET	3.5
1	A	1840	TYR	3.5
2	B	174	HIS	3.5
2	B	211[A]	GLN	3.5
1	A	1862	VAL	3.4
1	A	1901	GLY	3.3
2	B	43	VAL	3.3
2	B	132	LYS	3.3
1	A	2059	ILE	3.3
2	B	77	LEU	3.2
1	A	2017[A]	THR	3.2
2	B	55[A]	ARG	3.2
2	B	208	VAL	3.2
1	A	2049	ILE	3.2
2	B	152	LEU	3.2
2	B	81	MET	3.1
1	A	2041	PRO	3.1
1	A	1961[A]	LEU	3.1
2	B	92	ILE	3.1
2	B	246	MET	3.1
1	A	1904	ARG	3.1
2	B	275	LEU	3.0
1	A	1870	VAL	3.0
1	A	2001[A]	SER	3.0
2	B	126	ILE	3.0
2	B	41[A]	VAL	3.0
1	A	1956	ILE	3.0
1	A	1888	HIS	3.0
1	A	1837	SER	2.9
2	B	173	ALA	2.9
2	B	315	GLU	2.9
1	A	1965	PHE	2.9
2	B	67	PHE	2.9
2	B	189	ILE	2.9
2	B	51	ASN	2.9
2	B	95	ASN	2.9
2	B	127	ARG	2.8
1	A	2051	ILE	2.8
2	B	46	PHE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	18	ASP	2.8
2	B	281	ASP	2.8
2	B	196	GLU	2.8
1	A	2042	SER	2.8
1	A	1909	ALA	2.7
2	B	254	ALA	2.7
1	A	2043	PHE	2.7
2	B	267	ILE	2.7
1	A	2018[A]	ASN	2.7
2	B	192	GLY	2.7
1	A	1960[A]	GLU	2.7
2	B	282	ILE	2.7
2	B	49	ALA	2.7
1	A	1913	THR	2.6
2	B	214	PHE	2.6
1	A	1966	SER	2.6
2	B	274	THR	2.6
1	A	2057[A]	ASP	2.6
2	B	294	TYR	2.6
1	A	2031	THR	2.6
2	B	50	ASP	2.6
1	A	1940	MET	2.6
2	B	89	PHE	2.5
2	B	106	PRO	2.5
1	A	1962	ARG	2.5
1	A	1979[A]	MET	2.5
1	A	1848	ILE	2.5
1	A	1846	ASN	2.5
1	A	2062	GLU	2.5
1	A	2047	GLN	2.5
2	B	221	PHE	2.5
2	B	2	ASN	2.5
1	A	2023	LYS	2.4
2	B	87	ALA	2.4
2	B	222	GLY	2.4
1	A	1953	ASN	2.4
1	A	1865	THR	2.4
2	B	297	PHE	2.4
2	B	177[A]	ASN	2.4
2	B	317	LEU	2.4
2	B	146	THR	2.4
2	B	4	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1941	LEU	2.4
1	A	1894	ILE	2.4
2	B	278	GLN	2.4
2	B	44[A]	ILE	2.4
2	B	42[A]	HIS	2.3
1	A	1997	ASP	2.3
1	A	1977	VAL	2.3
2	B	264	LEU	2.3
2	B	28	GLN	2.3
1	A	2061	THR	2.3
1	A	1878	CYS	2.3
1	A	2002[A]	TYR	2.3
2	B	308	ILE	2.2
2	B	213	ILE	2.2
1	A	1861	THR	2.2
1	A	2033	THR	2.2
2	B	217	SER	2.2
1	A	1954	ILE	2.2
2	B	128	LYS	2.2
1	A	1998	ARG	2.2
2	B	23	ASN	2.2
2	B	114	TRP	2.2
1	A	2005	PHE	2.1
2	B	226	PHE	2.1
2	B	228	PHE	2.1
2	B	175	SER	2.1
1	A	1950	ASP	2.1
1	A	1976	ASP	2.1
1	A	2009	THR	2.0
1	A	1918[A]	SER	2.0
1	A	2021	SER	2.0
2	B	9	ALA	2.0
1	A	1944	LEU	2.0
1	A	2058	LEU	2.0
1	A	1931[A]	LYS	2.0
2	B	14	THR	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 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
3	V3R	B	401	13/13	0.88	0.31	20,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.