



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2021 – 12:19 PM JST

PDB ID : 7E5M  
Title : crystal structure of trans assembled human TROP-2  
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Deposited on : 2021-02-19  
Resolution : 3.20 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.

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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 : 2.24  
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) : 2.24

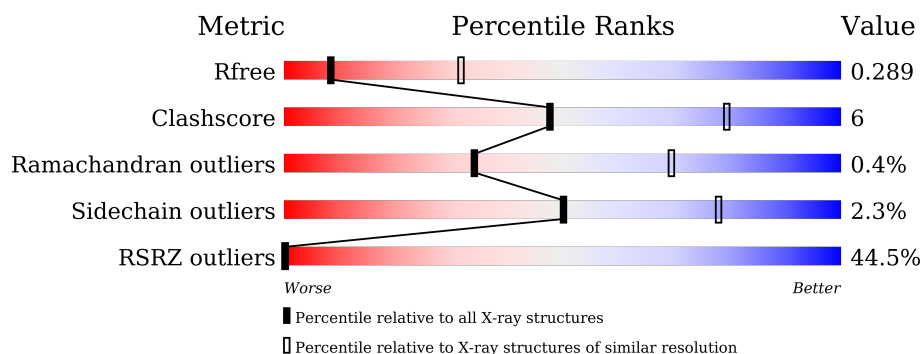
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	236	<div> <div>48%</div> <div>84%</div> <div>15%</div> </div>
1	B	236	<div> <div>41%</div> <div>80%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	301	-	-	-	X
2	NAG	B	301	-	-	-	X

## 2 Entry composition [i](#)

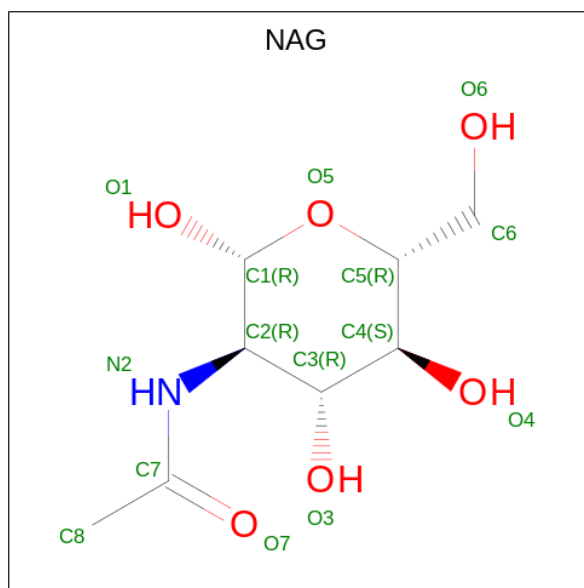
There are 2 unique types of molecules in this entry. The entry contains 3690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tumor-associated calcium signal transducer 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1844	1138	344	347	15			
1	B	236	Total	C	N	O	S	0	0	0
			1818	1123	336	344	15			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

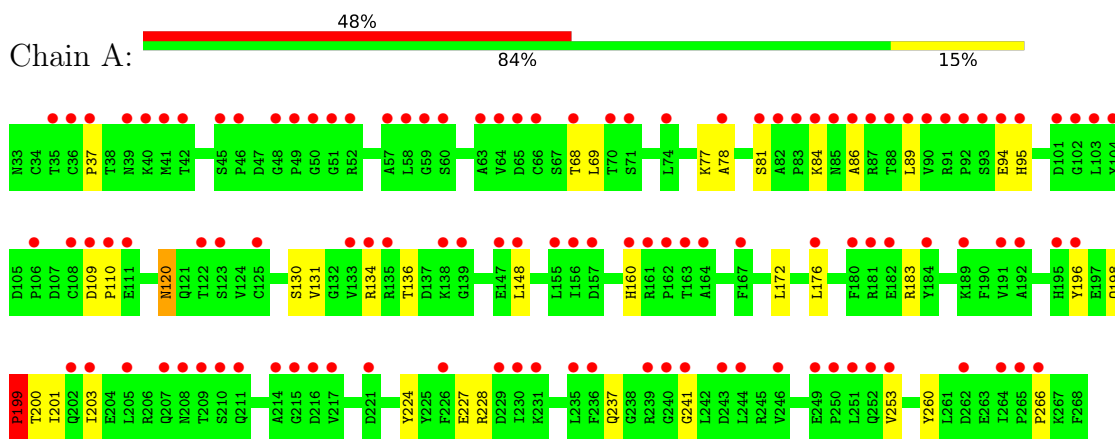


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

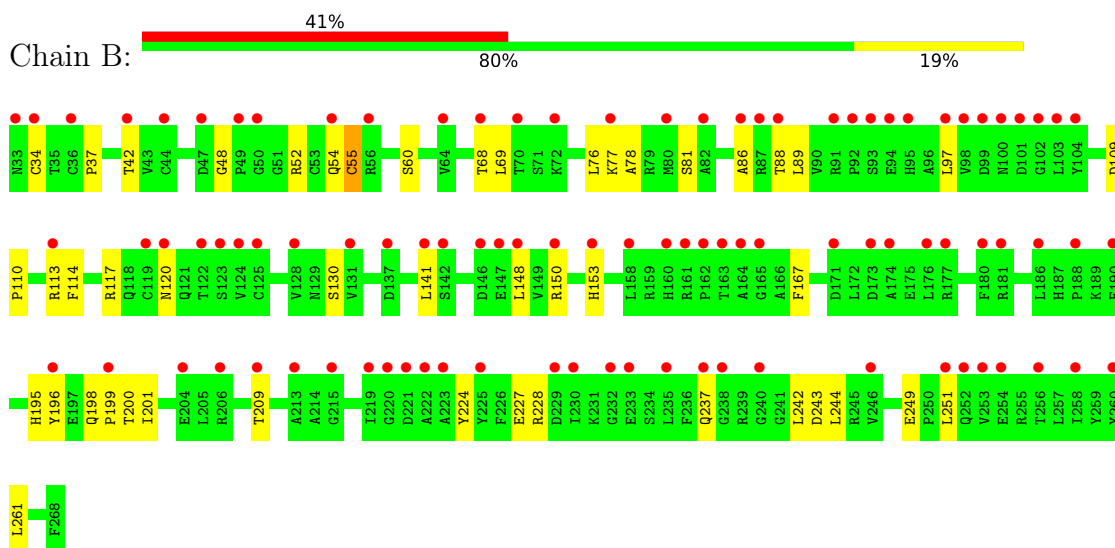
### 3 Residue-property plots [i](#)

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: Tumor-associated calcium signal transducer 2



- Molecule 1: Tumor-associated calcium signal transducer 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.54Å 126.88Å 54.07Å 90.00° 118.39° 90.00°	Depositor
Resolution (Å)	45.34 – 3.20 45.34 – 3.19	Depositor EDS
% Data completeness (in resolution range)	77.4 (45.34-3.20) 77.3 (45.34-3.19)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	80.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.239 , 0.283 0.243 , 0.289	Depositor DCC
$R_{free}$ test set	402 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.389 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	3690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.26	0/1879	0.57	0/2541
1	B	0.25	0/1853	0.55	0/2510
All	All	0.26	0/3732	0.56	0/5051

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

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	1844	0	1797	20	0
1	B	1818	0	1747	25	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0
All	All	3690	0	3570	44	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 6.

All (44) 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:B:198:GLN:O	1:B:200:THR:N	2.16	0.77
1:A:120:ASN:HD22	2:A:301:NAG:C7	2.07	0.67
1:A:37:PRO:HA	1:A:237:GLN:HB2	1.81	0.63
1:A:86:ALA:HB1	1:A:89:LEU:HB2	1.84	0.59
1:B:120:ASN:HD22	2:B:301:NAG:C7	2.18	0.56
1:B:224:TYR:HA	1:B:227:GLU:HG2	1.87	0.55
1:B:167:PHE:HE1	1:B:249:GLU:HG2	1.72	0.55
1:B:242:LEU:HG	1:B:244:LEU:HB2	1.92	0.52
1:B:150:ARG:HD3	1:B:209:THR:HG22	1.91	0.51
1:A:130:SER:HA	1:A:148:LEU:HD21	1.92	0.51
1:B:130:SER:HA	1:B:148:LEU:HD21	1.93	0.51
1:A:109:ASP:HB2	1:A:110:PRO:HD2	1.91	0.51
1:A:131:VAL:HG21	1:A:260:TYR:CE1	2.46	0.50
1:B:244:LEU:HG	1:B:251:LEU:HB3	1.94	0.50
1:A:160:HIS:HA	1:A:253:VAL:HA	1.93	0.49
1:A:198:GLN:O	1:A:200:THR:N	2.46	0.49
1:A:266:PRO:HG3	1:B:195:HIS:HE1	1.77	0.49
1:B:153:HIS:HB3	1:B:261:LEU:HB3	1.95	0.48
1:A:224:TYR:O	1:A:228:ARG:HG2	2.14	0.48
1:B:48:GLY:HA3	1:B:52:ARG:HB3	1.96	0.47
1:A:94:GLU:HG3	1:A:95:HIS:ND1	2.30	0.46
1:B:224:TYR:O	1:B:228:ARG:HG2	2.16	0.46
1:B:37:PRO:HA	1:B:237:GLN:HB2	1.97	0.46
1:B:86:ALA:O	1:B:88:THR:N	2.49	0.45
1:A:224:TYR:HA	1:A:227:GLU:HG2	1.99	0.45
1:A:196:TYR:CD1	1:A:201:ILE:HG12	2.53	0.44
1:A:68:THR:OG1	1:A:69:LEU:N	2.51	0.44
1:A:183:ARG:NH2	1:A:241:GLY:O	2.46	0.43
1:B:76:LEU:HD12	1:B:114:PHE:HZ	1.83	0.43
1:B:109:ASP:HB2	1:B:110:PRO:HD2	2.01	0.43
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.83	0.43
1:B:196:TYR:CD1	1:B:201:ILE:HG12	2.54	0.43
1:A:172:LEU:HD21	1:A:201:ILE:HD13	2.00	0.42
1:B:48:GLY:HA2	1:B:54:GLN:NE2	2.35	0.42
1:A:78:ALA:O	1:A:81:SER:HB3	2.21	0.41
1:A:198:GLN:HG3	1:A:199:PRO:HD2	2.01	0.41
1:B:42:THR:HB	1:B:55:CYS:SG	2.60	0.41
1:A:134:ARG:HD2	1:A:136:THR:O	2.20	0.41
1:A:176:LEU:HD13	1:A:203:ILE:HD11	2.01	0.41
1:B:60:SER:HB3	1:B:77:LYS:HD3	2.02	0.41
1:B:68:THR:OG1	1:B:69:LEU:N	2.54	0.41
1:B:117:ARG:NH2	1:B:141:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ALA:HB1	1:B:89:LEU:HB2	2.03	0.40
1:B:78:ALA:O	1:B:81:SER:HB3	2.21	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	234/236 (99%)	216 (92%)	17 (7%)	1 (0%)	34	69
1	B	234/236 (99%)	218 (93%)	15 (6%)	1 (0%)	34	69
All	All	468/472 (99%)	434 (93%)	32 (7%)	2 (0%)	34	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PRO
1	B	199	PRO

### 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	201/203 (99%)	197 (98%)	4 (2%)	55	80
1	B	195/203 (96%)	190 (97%)	5 (3%)	46	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	396/406 (98%)	387 (98%)	9 (2%)	50 78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	84	LYS
1	A	120	ASN
1	A	199	PRO
1	B	34	CYS
1	B	55	CYS
1	B	97	LEU
1	B	113	ARG
1	B	243	ASP

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](#)

2 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	NAG	A	301	1	14,14,15	0.40	0	17,19,21	0.37	0
2	NAG	B	301	1	14,14,15	0.39	0	17,19,21	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	301	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAG	1	0
2	B	301	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.







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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	236/236 (100%)	2.66	114 (48%)  	27, 76, 163, 216	0
1	B	236/236 (100%)	2.25	96 (40%)  	27, 72, 164, 225	0
All	All	472/472 (100%)	2.45	210 (44%)  	27, 75, 164, 225	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	THR	17.9
1	B	253	VAL	17.5
1	A	82	ALA	16.6
1	A	86	ALA	13.2
1	A	81	SER	12.5
1	B	33	ASN	11.9
1	A	92	PRO	11.3
1	A	87	ARG	11.0
1	A	85	ASN	10.3
1	B	98	VAL	10.3
1	B	177	ARG	10.2
1	B	163	THR	9.8
1	B	102	GLY	9.6
1	A	50	GLY	9.4
1	B	95	HIS	9.0
1	A	59	GLY	8.9
1	B	164	ALA	8.8
1	B	99	ASP	8.7
1	B	254	GLU	8.4
1	B	94	GLU	8.3
1	B	252	GLN	8.1
1	A	41	MET	8.0
1	A	111	GLU	7.9
1	A	91	ARG	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLN	7.5
1	A	161	ARG	7.2
1	A	52	ARG	7.0
1	A	39	ASN	6.8
1	B	103	LEU	6.7
1	A	109	ASP	6.6
1	A	95	HIS	6.5
1	A	108	CYS	6.4
1	A	83	PRO	6.4
1	A	51	GLY	6.4
1	A	89	LEU	6.3
1	B	160	HIS	6.0
1	A	239	ARG	5.9
1	B	176	LEU	5.8
1	A	211	GLN	5.8
1	A	133	VAL	5.7
1	A	90	VAL	5.6
1	B	49	PRO	5.4
1	A	49	PRO	5.4
1	A	240	GLY	5.4
1	B	220	GLY	5.4
1	B	101	ASP	5.3
1	B	256	THR	5.3
1	A	214	ALA	5.3
1	A	207	GLN	5.3
1	A	162	PRO	5.2
1	A	110	PRO	5.1
1	B	93	SER	5.1
1	B	100	ASN	5.1
1	A	251	LEU	5.0
1	A	60	SER	5.0
1	A	101	ASP	4.9
1	A	210	SER	4.9
1	A	147	GLU	4.9
1	A	106	PRO	4.9
1	B	240	GLY	4.8
1	B	119	CYS	4.8
1	B	92	PRO	4.8
1	A	93	SER	4.7
1	A	71	SER	4.6
1	A	264	ILE	4.6
1	B	56	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	238	GLY	4.6
1	A	230	ILE	4.5
1	A	249	GLU	4.5
1	B	137	ASP	4.4
1	A	243	ASP	4.3
1	B	150	ARG	4.3
1	B	223	ALA	4.3
1	A	265	PRO	4.2
1	B	219	ILE	4.2
1	B	258	ILE	4.2
1	B	233	GLU	4.2
1	A	40	LYS	4.2
1	A	94	GLU	4.2
1	A	157	ASP	4.2
1	B	125	CYS	4.1
1	A	181	ARG	4.1
1	B	142	SER	4.0
1	A	123	SER	4.0
1	B	161	ARG	4.0
1	A	35	THR	3.9
1	A	167	PHE	3.9
1	B	229	ASP	3.9
1	B	123	SER	3.9
1	B	91	ARG	3.9
1	B	206	ARG	3.9
1	B	141	LEU	3.9
1	A	217	VAL	3.9
1	A	138	LYS	3.8
1	B	68	THR	3.8
1	B	122	THR	3.8
1	B	124	VAL	3.7
1	A	180	PHE	3.7
1	A	102	GLY	3.7
1	A	163	THR	3.7
1	B	77	LYS	3.6
1	A	74	LEU	3.6
1	A	148	LEU	3.6
1	A	63	ALA	3.6
1	B	153	HIS	3.6
1	A	244	LEU	3.6
1	A	246	VAL	3.6
1	A	250	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	195	HIS	3.5
1	A	226	PHE	3.5
1	A	191	VAL	3.4
1	B	196	TYR	3.3
1	B	146	ASP	3.3
1	B	72	LYS	3.3
1	B	87	ARG	3.3
1	A	192	ALA	3.3
1	B	162	PRO	3.3
1	B	199	PRO	3.3
1	B	148	LEU	3.2
1	A	208	ASN	3.2
1	B	70	THR	3.2
1	A	253	VAL	3.1
1	B	260	TYR	3.1
1	A	236	PHE	3.1
1	B	188	PRO	3.1
1	B	237	GLN	3.1
1	B	82	ALA	3.0
1	B	113	ARG	3.0
1	A	215	GLY	3.0
1	B	173	ASP	2.9
1	A	202	GLN	2.9
1	B	50	GLY	2.9
1	B	88	THR	2.9
1	A	164	ALA	2.9
1	A	58	LEU	2.9
1	B	80	MET	2.9
1	B	147	GLU	2.9
1	B	225	TYR	2.8
1	A	266	PRO	2.8
1	B	165	GLY	2.8
1	A	262	ASP	2.8
1	B	97	LEU	2.8
1	B	104	TYR	2.8
1	A	155	LEU	2.7
1	A	104	TYR	2.7
1	A	65	ASP	2.7
1	A	176	LEU	2.7
1	B	209	THR	2.7
1	A	64	VAL	2.7
1	B	42	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	171	ASP	2.7
1	B	180	PHE	2.6
1	A	229	ASP	2.6
1	A	189	LYS	2.6
1	B	34	CYS	2.6
1	A	135	ARG	2.6
1	A	241	GLY	2.6
1	A	203	ILE	2.6
1	A	48	GLY	2.6
1	B	215	GLY	2.6
1	B	251	LEU	2.6
1	B	213	ALA	2.5
1	A	46	PRO	2.5
1	B	131	VAL	2.5
1	A	221	ASP	2.5
1	B	64	VAL	2.4
1	A	122	THR	2.4
1	B	221	ASP	2.4
1	B	190	PHE	2.4
1	B	158	LEU	2.4
1	A	68	THR	2.4
1	A	66	CYS	2.4
1	A	125	CYS	2.4
1	A	84	LYS	2.4
1	A	103	LEU	2.4
1	B	120	ASN	2.3
1	B	36	CYS	2.3
1	B	47	ASP	2.3
1	A	156	ILE	2.3
1	A	45	SER	2.3
1	A	182	GLU	2.3
1	A	42	THR	2.3
1	A	205	LEU	2.3
1	A	235	LEU	2.3
1	B	235	LEU	2.3
1	A	231	LYS	2.3
1	B	246	VAL	2.3
1	A	139	GLY	2.3
1	B	181	ARG	2.3
1	A	184	TYR	2.3
1	B	54	GLN	2.2
1	B	222	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	134	ARG	2.2
1	A	78	ALA	2.2
1	A	70	THR	2.2
1	B	186	LEU	2.2
1	A	196	TYR	2.2
1	B	232	GLY	2.1
1	A	57	ALA	2.1
1	A	36	CYS	2.1
1	B	204	GLU	2.1
1	A	160	HIS	2.1
1	A	209	THR	2.1
1	B	174	ALA	2.1
1	B	86	ALA	2.1
1	B	128	VAL	2.1
1	B	230	ILE	2.0
1	A	216	ASP	2.0
1	B	44	CYS	2.0
1	A	37	PRO	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<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
2	NAG	B	301	14/15	0.41	0.47	62,65,73,82	0
2	NAG	A	301	14/15	0.64	0.45	85,98,101,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.