



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:14 am BST

PDB ID : 3BJI  
Title : Structural Basis of Promiscuous Guanine Nucleotide Exchange by the T-Cell Essential Vav1  
Authors : Chrencik, J.E.; Brooun, A.; Kuhn, P.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)  
Deposited on : 2007-12-04  
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

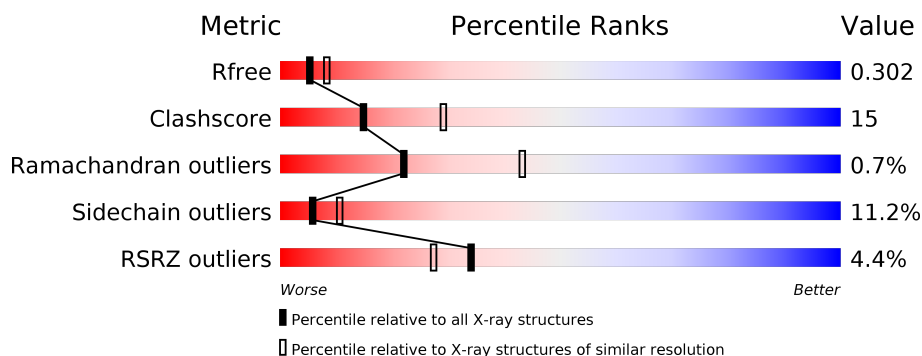
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	378	<div> <div>63%</div> <div>28%</div> <div>7%</div> <div>•</div> </div>
1	B	378	<div> <div>63%</div> <div>26%</div> <div>6%</div> <div>• •</div> </div>
2	C	177	<div>10%</div> <div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
2	D	177	<div>12%</div> <div> <div>62%</div> <div>24%</div> <div>6%</div> <div>• 7%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8423 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 Proto-oncogene vav.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2937	1863	504	544	26			
1	B	368	Total	C	N	O	S	0	0	0
			2914	1853	503	532	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	GLY	-	EXPRESSION TAG	UNP P15498
B	566	GLY	-	EXPRESSION TAG	UNP P15498

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1305	838	214	246	7			
2	D	164	Total	C	N	O	S	0	0	0
			1203	773	196	228	6			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

*Continued on next page...*

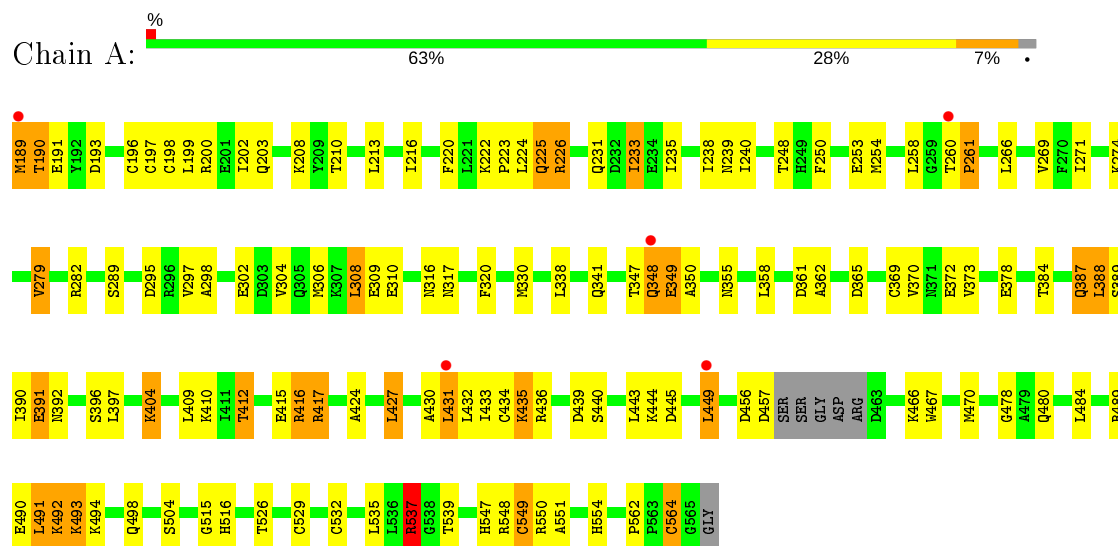
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	O 3	0	0
4	C	14	Total 14	O 14	0	0
4	D	8	Total 8	O 8	0	0

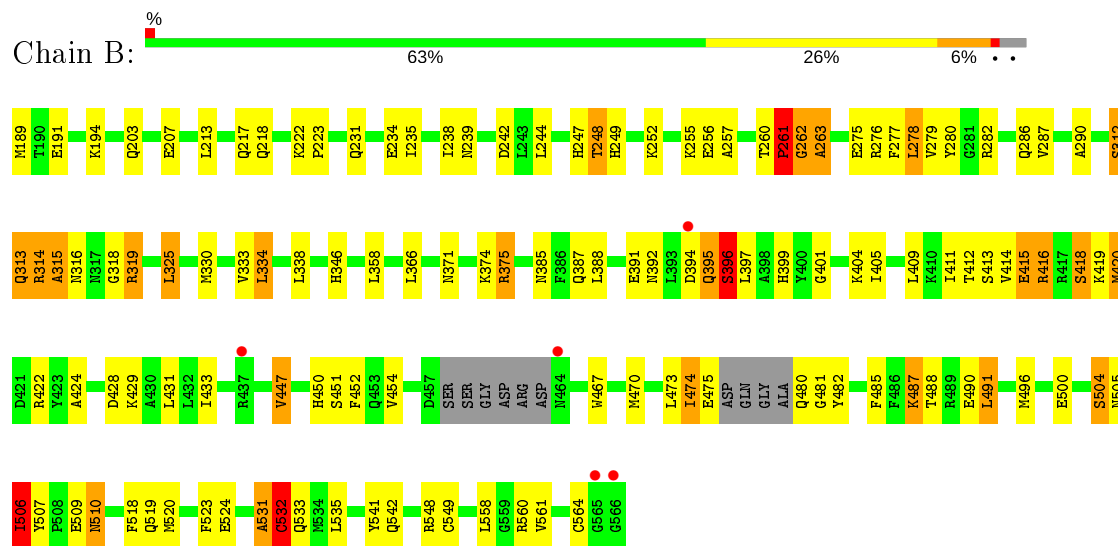
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Proto-oncogene vav

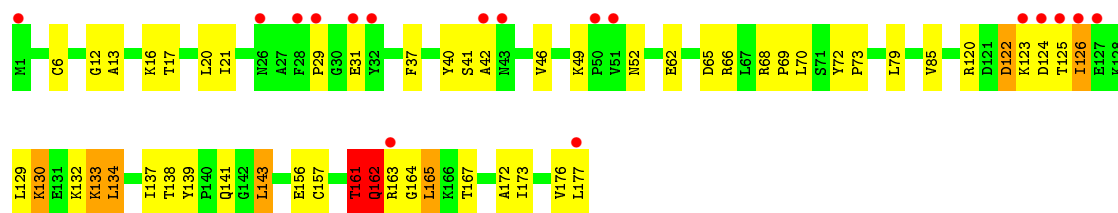


#### • Molecule 1: Proto-oncogene vav

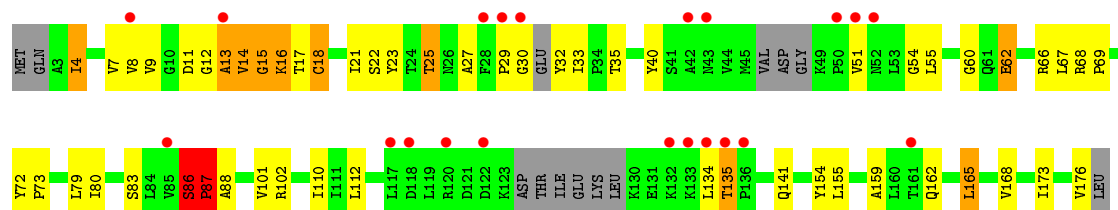


#### • Molecule 2: Ras-related C3 botulinum toxin substrate 1 precursor





- Molecule 2: Ras-related C3 botulinum toxin substrate 1 precursor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.95Å 75.08Å 114.86Å 90.00° 103.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 28.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.60) 94.4 (28.55-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	33.28 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.221 , 0.293 0.230 , 0.302	Depositor DCC
$R_{free}$ test set	1939 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: ZN

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	3/2991 (0.1%)	0.97	14/4030 (0.3%)
1	B	0.77	0/2967	0.88	8/3996 (0.2%)
2	C	0.71	0/1334	0.81	3/1828 (0.2%)
2	D	0.51	0/1229	0.77	4/1683 (0.2%)
All	All	0.73	3/8521 (0.0%)	0.88	29/11537 (0.3%)

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
1	A	0	8
1	B	0	14
2	C	0	2
2	D	0	2
All	All	0	26

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	CYS	CB-SG	-11.01	1.63	1.82
1	A	196	CYS	CB-SG	-5.86	1.72	1.81
1	A	434	CYS	CB-SG	-5.50	1.72	1.81

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	CYS	N-CA-CB	-22.93	69.33	110.60
1	A	416	ARG	N-CA-C	12.81	145.58	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	14	VAL	CB-CA-C	-11.07	90.36	111.40
1	A	417	ARG	N-CA-CB	-9.44	93.61	110.60
1	B	416	ARG	N-CA-CB	8.45	125.80	110.60
1	B	506	ILE	N-CA-C	-8.03	89.33	111.00
1	A	493	LYS	N-CA-C	-7.91	89.65	111.00
2	C	29	PRO	CB-CA-C	-7.68	92.79	112.00
1	A	226	ARG	N-CA-C	-7.62	90.43	111.00
1	B	396	SER	N-CA-C	-7.34	91.18	111.00
2	D	86	SER	C-N-CD	-7.21	104.73	120.60
2	C	162	GLN	N-CA-C	7.09	130.15	111.00
1	A	392	ASN	N-CA-C	-7.05	91.97	111.00
1	A	350	ALA	N-CA-C	6.32	128.06	111.00
1	A	549	CYS	CB-CA-C	-6.25	97.91	110.40
1	B	375	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	198	CYS	N-CA-C	6.00	127.19	111.00
1	A	416	ARG	CB-CA-C	-6.00	98.40	110.40
1	B	394	ASP	CB-CA-C	5.97	122.34	110.40
2	D	86	SER	C-N-CA	5.73	146.05	122.00
1	A	196	CYS	CB-CA-C	-5.67	99.06	110.40
1	A	537	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	564	CYS	CA-CB-SG	5.61	124.10	114.00
1	B	474	ILE	CB-CA-C	-5.51	100.57	111.60
1	A	197	CYS	N-CA-C	5.51	125.88	111.00
2	C	161	THR	C-N-CA	-5.43	108.12	121.70
1	B	549	CYS	N-CA-C	-5.27	96.76	111.00
1	B	415	GLU	N-CA-C	-5.15	97.10	111.00
2	D	15	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	GLN	Peptide
1	A	349	GLU	Peptide
1	A	390	ILE	Peptide
1	A	391	GLU	Peptide
1	A	416	ARG	Peptide
1	A	435	LYS	Peptide
1	A	478	GLY	Peptide
1	A	492	LYS	Peptide
1	B	261	PRO	Peptide
1	B	262	GLY	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	263	ALA	Peptide
1	B	313	GLN	Peptide
1	B	314	ARG	Peptide
1	B	315	ALA	Peptide
1	B	392	ASN	Peptide
1	B	395	GLN	Peptide
1	B	396	SER	Peptide
1	B	420	MET	Peptide
1	B	505	ASN	Peptide
1	B	510	ASN	Peptide
1	B	531	ALA	Peptide
1	B	532	CYS	Peptide
2	C	130	LYS	Peptide
2	C	161	THR	Peptide
2	D	13	ALA	Peptide
2	D	86	SER	Peptide

## 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	2937	0	2793	70	0
1	B	2914	0	2780	92	0
2	C	1305	0	1247	47	0
2	D	1203	0	1113	48	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	35	0	0	1	0
4	B	3	0	0	0	0
4	C	14	0	0	0	0
4	D	8	0	0	1	0
All	All	8423	0	7933	248	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 15.

All (248) 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:C:162:GLN:HB2	2:C:165:LEU:HB2	1.29	1.13
2:D:14:VAL:HG12	2:D:15:GLY:N	1.61	1.08
1:A:549:CYS:SG	1:A:564:CYS:HB3	1.94	1.07
1:B:488:THR:HG22	1:B:490:GLU:N	1.73	1.03
2:C:162:GLN:CB	2:C:165:LEU:HB2	1.89	1.02
1:B:244:LEU:O	1:B:248:THR:HG23	1.60	1.01
1:B:315:ALA:N	1:B:316:ASN:HA	1.72	1.01
2:C:120:ARG:O	2:C:126:ILE:HD11	1.65	0.97
2:D:80:ILE:HD13	2:D:110:ILE:HG23	1.48	0.95
2:D:8:VAL:HG12	2:D:16:LYS:HG2	1.49	0.95
1:A:199:LEU:HD22	1:A:258:LEU:HD11	1.47	0.94
1:B:314:ARG:C	1:B:316:ASN:HA	1.87	0.93
2:D:14:VAL:HG12	2:D:15:GLY:H	1.28	0.91
2:C:162:GLN:HB2	2:C:165:LEU:CB	2.02	0.88
1:B:474:ILE:HG22	1:B:475:GLU:O	1.76	0.84
1:B:404:LYS:O	1:B:405:ILE:HG23	1.80	0.81
1:B:488:THR:HG21	1:B:490:GLU:CB	2.11	0.80
1:B:315:ALA:N	1:B:316:ASN:CA	2.45	0.80
2:D:14:VAL:CG1	2:D:15:GLY:N	2.37	0.79
1:B:244:LEU:O	1:B:248:THR:CG2	2.31	0.79
2:C:129:LEU:HD22	2:C:134:LEU:HB3	1.66	0.77
1:B:315:ALA:O	1:B:319:ARG:CB	2.32	0.77
1:B:404:LYS:O	1:B:405:ILE:CG2	2.33	0.77
1:A:208:LYS:HD2	1:B:316:ASN:HD21	1.49	0.76
1:A:404:LYS:HB3	1:A:498:GLN:HE21	1.49	0.76
1:A:231:GLN:O	1:A:235:ILE:HG13	1.85	0.76
2:C:16:LYS:O	2:C:20:LEU:HD12	1.85	0.76
1:B:422:ARG:HD2	1:B:433:ILE:HG22	1.68	0.75
1:A:210:THR:HG21	1:A:248:THR:HG22	1.68	0.74
1:B:488:THR:CG2	1:B:490:GLU:CB	2.66	0.73
2:D:8:VAL:HG22	2:D:79:LEU:HD12	1.70	0.73
1:B:488:THR:CG2	1:B:490:GLU:N	2.52	0.73
2:D:80:ILE:HD13	2:D:110:ILE:CG2	2.18	0.72
1:A:397:LEU:HD21	1:A:432:LEU:HD11	1.71	0.72
1:A:258:LEU:HD13	1:A:266:LEU:HD13	1.70	0.71
2:D:51:VAL:HG21	2:D:173:ILE:HD13	1.72	0.71
1:B:333:VAL:HG13	1:B:334:LEU:HD13	1.71	0.71
1:A:424:ALA:HB1	1:A:431:LEU:HD21	1.73	0.71
1:A:456:ASP:OD1	1:A:457:ASP:N	2.24	0.70
1:B:395:GLN:O	1:B:395:GLN:CD	2.30	0.70
1:B:315:ALA:O	1:B:319:ARG:HB2	1.92	0.70
1:A:370:VAL:HG12	2:D:67:LEU:HD11	1.74	0.69

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:THR:HG22	1:B:490:GLU:H	1.55	0.69
2:D:4:ILE:HG22	2:D:4:ILE:O	1.92	0.69
2:D:155:LEU:HD12	2:D:168:VAL:HG22	1.74	0.68
1:A:537:ARG:HG3	1:A:537:ARG:HH11	1.60	0.67
2:C:122:ASP:OD1	2:C:125:THR:N	2.27	0.67
2:D:14:VAL:CG1	2:D:15:GLY:H	2.00	0.66
1:B:474:ILE:HG22	1:B:475:GLU:N	2.09	0.66
1:B:395:GLN:N	1:B:395:GLN:OE1	2.29	0.66
1:B:488:THR:CG2	1:B:490:GLU:H	2.08	0.65
1:B:313:GLN:N	1:B:313:GLN:OE1	2.30	0.65
2:C:164:GLY:O	2:C:167:THR:N	2.30	0.65
2:C:40:TYR:OH	2:C:42:ALA:HB3	1.97	0.64
1:B:371:ASN:OD1	2:C:66:ARG:HB2	1.96	0.64
2:D:13:ALA:HA	2:D:14:VAL:O	1.96	0.64
1:A:222:LYS:HA	1:A:225:GLN:HG3	1.79	0.63
2:C:162:GLN:HB3	2:C:165:LEU:CD2	2.28	0.63
1:B:467:TRP:CZ2	1:B:487:LYS:HG2	2.34	0.63
1:B:315:ALA:O	1:B:319:ARG:HB3	1.98	0.62
1:B:275:GLU:HA	1:B:278:LEU:HD22	1.80	0.62
2:D:13:ALA:CA	2:D:14:VAL:O	2.47	0.61
1:A:387:GLN:O	1:A:391:GLU:HG3	2.01	0.61
2:C:162:GLN:CB	2:C:165:LEU:CB	2.70	0.61
1:A:529:CYS:HB2	1:A:554:HIS:CE1	2.36	0.60
2:C:17:THR:HG22	2:C:21:ILE:HD12	1.83	0.60
1:B:480:GLN:CG	1:B:481:GLY:N	2.64	0.60
1:B:244:LEU:HD12	1:B:248:THR:HG22	1.85	0.59
2:D:80:ILE:CD1	2:D:110:ILE:HG23	2.28	0.59
1:B:488:THR:HG22	1:B:490:GLU:CA	2.33	0.58
2:C:122:ASP:OD1	2:C:123:LYS:N	2.36	0.58
1:B:480:GLN:CG	1:B:481:GLY:H	2.16	0.58
2:C:161:THR:CB	2:C:162:GLN:HA	2.33	0.58
2:C:162:GLN:HB3	2:C:165:LEU:HD22	1.86	0.57
1:A:410:LYS:HE3	1:A:467:TRP:CD2	2.38	0.57
2:D:12:GLY:O	2:D:13:ALA:C	2.43	0.57
2:C:162:GLN:HB3	2:C:165:LEU:HB2	1.80	0.57
1:B:387:GLN:OE1	1:B:397:LEU:N	2.31	0.57
2:D:23:TYR:HB2	2:D:165:LEU:HD11	1.87	0.57
1:A:223:PRO:O	1:A:226:ARG:CB	2.53	0.56
1:A:239:ASN:ND2	1:A:279:VAL:HG13	2.20	0.56
2:C:122:ASP:OD1	2:C:124:ASP:N	2.37	0.56
1:A:456:ASP:O	1:A:457:ASP:CB	2.53	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:GLU:O	2:C:157:CYS:HB3	2.06	0.56
1:A:302:GLU:O	1:A:306:MET:HG2	2.07	0.55
1:A:373:VAL:HG22	1:A:539:THR:HG23	1.89	0.55
1:A:397:LEU:CD2	1:A:432:LEU:HD11	2.36	0.55
1:B:447:VAL:HG23	1:B:452:PHE:CE2	2.41	0.55
1:A:489:ARG:O	1:A:493:LYS:HB2	2.07	0.55
2:D:54:GLY:O	2:D:55:LEU:HD23	2.06	0.55
1:B:488:THR:HG22	1:B:491:LEU:H	1.71	0.55
2:D:7:VAL:HG12	2:D:9:VAL:CG1	2.37	0.55
1:B:500:GLU:O	1:B:504:SER:HB3	2.07	0.54
2:C:85:VAL:HG12	2:C:85:VAL:O	2.07	0.54
1:A:189:MET:N	4:A:570:HOH:O	2.40	0.54
1:B:314:ARG:O	1:B:316:ASN:HA	2.05	0.54
1:B:488:THR:HB	1:B:491:LEU:HB2	1.90	0.54
1:B:496:MET:O	1:B:500:GLU:HG3	2.07	0.54
1:A:430:ALA:CA	1:A:449:LEU:HD22	2.38	0.54
2:D:40:TYR:HD1	4:D:179:HOH:O	1.90	0.54
1:B:424:ALA:HB1	1:B:431:LEU:HD11	1.89	0.54
1:A:210:THR:CG2	1:A:248:THR:HG22	2.35	0.54
1:A:316:ASN:OD1	1:A:320:PHE:N	2.40	0.54
2:D:21:ILE:O	2:D:25:THR:HB	2.08	0.54
1:A:491:LEU:O	1:A:492:LYS:C	2.45	0.53
1:B:413:SER:OG	1:B:414:VAL:N	2.38	0.53
2:D:18:CYS:SG	2:D:33:ILE:HG21	2.48	0.53
1:A:271:ILE:HD11	1:A:358:LEU:HD23	1.89	0.53
1:B:474:ILE:CG2	1:B:475:GLU:N	2.71	0.53
2:D:155:LEU:HD12	2:D:168:VAL:CG2	2.40	0.52
1:B:488:THR:HB	1:B:491:LEU:HD22	1.92	0.52
1:A:424:ALA:HB1	1:A:431:LEU:CD2	2.39	0.52
2:D:155:LEU:HD12	2:D:168:VAL:HA	1.90	0.52
1:B:203:GLN:NE2	1:B:207:GLU:OE2	2.41	0.51
1:B:412:THR:HG22	1:B:419:LYS:N	2.25	0.51
1:B:189:MET:HE3	2:C:31:GLU:C	2.31	0.51
2:D:83:SER:O	2:D:86:SER:O	2.28	0.51
1:B:316:ASN:OD1	1:B:316:ASN:O	2.30	0.50
2:C:161:THR:CB	2:C:163:ARG:N	2.74	0.50
2:D:154:TYR:O	2:D:155:LEU:HD23	2.12	0.50
2:D:8:VAL:CG1	2:D:16:LYS:HG2	2.31	0.50
1:B:276:ARG:HH12	1:B:279:VAL:HG21	1.76	0.50
1:A:435:LYS:HB2	1:A:444:LYS:HD2	1.93	0.50
2:D:87:PRO:O	2:D:88:ALA:C	2.49	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASN:ND2	1:B:279:VAL:HG13	2.26	0.50
1:B:277:PHE:HB3	1:B:366:LEU:HD21	1.92	0.50
2:C:20:LEU:HD22	2:C:37:PHE:CE2	2.47	0.49
1:A:260:THR:CB	1:A:261:PRO:CD	2.91	0.48
2:C:40:TYR:CZ	2:C:42:ALA:HB3	2.47	0.48
2:D:87:PRO:CG	2:D:134:LEU:HD22	2.43	0.48
1:B:257:ALA:O	1:B:263:ALA:HB1	2.13	0.48
2:D:87:PRO:HG3	2:D:134:LEU:HD22	1.95	0.48
1:A:274:LYS:HD2	1:A:362:ALA:HB1	1.96	0.48
1:A:389:SER:O	1:A:389:SER:OG	2.29	0.48
1:B:467:TRP:CH2	1:B:487:LYS:HG2	2.49	0.48
2:D:30:GLY:HA2	2:D:32:TYR:N	2.28	0.48
1:B:395:GLN:CG	1:B:395:GLN:O	2.56	0.48
1:B:518:PHE:CD2	1:B:558:LEU:HD22	2.49	0.48
1:A:427:LEU:N	1:A:427:LEU:HD23	2.29	0.48
1:B:244:LEU:HD12	1:B:248:THR:CG2	2.43	0.47
1:B:412:THR:HG22	1:B:418:SER:C	2.33	0.47
1:A:537:ARG:HH11	1:A:537:ARG:CG	2.26	0.47
2:D:51:VAL:HG21	2:D:173:ILE:CD1	2.42	0.47
1:A:258:LEU:CD1	1:A:266:LEU:HD13	2.42	0.47
1:B:401:GLY:HA2	1:B:541:TYR:CE2	2.49	0.47
1:A:295:ASP:O	1:A:298:ALA:HB3	2.15	0.47
1:B:231:GLN:O	1:B:235:ILE:HG13	2.15	0.47
1:B:487:LYS:H	1:B:487:LYS:HG3	1.47	0.47
2:D:7:VAL:HG12	2:D:9:VAL:HG12	1.96	0.47
1:A:338:LEU:HD11	2:D:60:GLY:N	2.30	0.46
1:B:252:LYS:O	1:B:256:GLU:HG3	2.15	0.46
1:A:470:MET:HA	1:A:484:LEU:O	2.16	0.46
2:C:139:TYR:CE2	2:C:143:LEU:HD22	2.51	0.46
2:C:72:TYR:N	2:C:73:PRO:CD	2.79	0.46
1:B:312:SER:HB3	1:B:318:GLY:HA2	1.97	0.46
1:A:224:LEU:HD11	1:A:308:LEU:CD1	2.46	0.46
2:D:60:GLY:N	2:D:62:GLU:OE2	2.43	0.45
1:A:250:PHE:CE1	1:A:269:VAL:HG12	2.51	0.45
1:A:297:VAL:HG12	1:A:304:VAL:HG11	1.98	0.45
2:D:4:ILE:HG12	2:D:176:VAL:HG11	1.98	0.45
1:B:506:ILE:HG22	1:B:507:TYR:CD2	2.52	0.45
1:B:222:LYS:HB2	1:B:223:PRO:HD3	1.99	0.45
1:B:531:ALA:HB3	1:B:532:CYS:HB3	1.98	0.45
1:B:217:GLN:OE1	1:B:218:GLN:NE2	2.49	0.45
2:D:135:THR:HG21	2:D:141:GLN:HE22	1.79	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:THR:HG21	2:D:35:THR:O	2.16	0.45
1:A:549:CYS:O	1:A:550:ARG:CG	2.64	0.45
1:A:516:HIS:NE2	1:A:562:PRO:O	2.49	0.45
2:D:25:THR:HG22	2:D:27:ALA:O	2.17	0.45
1:B:282:ARG:NE	1:B:286:GLN:OE1	2.47	0.45
2:C:12:GLY:O	2:C:13:ALA:HB3	2.15	0.45
2:D:68:ARG:HG3	2:D:69:PRO:HD3	1.99	0.45
2:C:176:VAL:O	2:C:177:LEU:CB	2.64	0.45
1:B:414:VAL:C	1:B:415:GLU:O	2.52	0.44
1:B:429:LYS:NZ	1:B:541:TYR:OH	2.43	0.44
1:B:247:HIS:NE2	1:B:280:TYR:OH	2.29	0.44
2:C:46:VAL:HG21	2:C:173:ILE:HD13	1.99	0.44
1:B:415:GLU:O	1:B:416:ARG:C	2.54	0.44
2:C:137:ILE:N	2:C:137:ILE:HD13	2.32	0.44
1:A:190:THR:HB	1:A:193:ASP:H	1.83	0.44
1:A:216:ILE:O	1:A:220:PHE:HB2	2.17	0.44
2:C:85:VAL:O	2:C:85:VAL:CG1	2.65	0.44
2:D:22:SER:OG	2:D:159:ALA:HB1	2.18	0.44
1:A:189:MET:CE	2:D:32:TYR:N	2.81	0.44
1:A:430:ALA:HA	1:A:449:LEU:HD22	2.00	0.44
2:D:80:ILE:N	2:D:80:ILE:HD12	2.32	0.44
1:A:233:ILE:HD13	1:A:233:ILE:HG23	1.57	0.44
1:A:516:HIS:CE1	1:A:564:CYS:HB3	2.52	0.43
1:B:374:LYS:HZ3	2:C:70:LEU:HD21	1.83	0.43
1:A:433:ILE:HB	1:A:445:ASP:HB3	2.01	0.43
2:C:139:TYR:CE2	2:C:143:LEU:CD2	3.02	0.43
2:C:161:THR:CB	2:C:163:ARG:H	2.32	0.43
2:D:72:TYR:N	2:D:73:PRO:CD	2.81	0.43
2:C:68:ARG:HB2	2:C:69:PRO:HD3	2.00	0.43
1:A:369:CYS:SG	1:A:535:LEU:HD13	2.58	0.43
1:B:509:GLU:O	1:B:510:ASN:HB2	2.19	0.43
1:B:548:ARG:HB2	1:B:564:CYS:SG	2.59	0.43
2:D:27:ALA:N	2:D:162:GLN:HE22	2.16	0.43
1:A:549:CYS:SG	1:A:564:CYS:HB2	2.45	0.43
2:C:16:LYS:NZ	2:C:62:GLU:OE1	2.50	0.43
1:A:515:GLY:O	1:A:548:ARG:NH1	2.51	0.42
2:C:6:CYS:SG	2:C:79:LEU:HD13	2.59	0.42
2:D:112:LEU:HD23	2:D:154:TYR:CD1	2.54	0.42
2:C:122:ASP:CG	2:C:123:LYS:N	2.72	0.42
1:A:271:ILE:CD1	1:A:358:LEU:HD23	2.50	0.42
1:B:261:PRO:HA	1:B:262:GLY:HA2	1.60	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:HIS:O	1:B:541:TYR:OH	2.24	0.42
1:B:524:GLU:CG	1:B:524:GLU:O	2.67	0.42
1:B:470:MET:HG3	1:B:485:PHE:CZ	2.54	0.42
2:C:138:THR:H	2:C:141:GLN:HE21	1.67	0.42
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.82	0.42
1:A:412:THR:HG23	1:A:417:ARG:HA	2.02	0.42
1:B:401:GLY:HA2	1:B:541:TYR:CD2	2.55	0.42
1:B:488:THR:CG2	1:B:491:LEU:H	2.33	0.42
1:B:282:ARG:HG2	1:B:286:GLN:OE1	2.20	0.42
2:C:85:VAL:HG13	2:C:129:LEU:HD11	2.02	0.42
1:A:529:CYS:HB3	1:A:532:CYS:SG	2.59	0.42
1:B:375:ARG:NH2	2:C:65:ASP:OD2	2.52	0.42
1:A:202:ILE:HG22	1:A:254:MET:SD	2.60	0.41
1:A:466:LYS:O	1:A:467:TRP:HB2	2.21	0.41
1:B:239:ASN:HD22	1:B:279:VAL:HG13	1.85	0.41
2:C:138:THR:H	2:C:141:GLN:NE2	2.18	0.41
1:B:325:LEU:HA	1:B:325:LEU:HD12	1.83	0.41
2:C:122:ASP:OD1	2:C:122:ASP:C	2.59	0.41
2:C:46:VAL:O	2:C:49:LYS:N	2.54	0.41
1:B:488:THR:HB	1:B:491:LEU:CD2	2.50	0.41
1:B:523:PHE:HD2	1:B:542:GLN:HB2	1.85	0.41
1:A:378:GLU:OE1	2:D:66:ARG:HD3	2.20	0.41
2:C:172:ALA:O	2:C:176:VAL:HG23	2.20	0.41
1:B:452:PHE:HA	1:B:474:ILE:O	2.21	0.41
1:A:361:ASP:O	1:A:365:ASP:HB2	2.21	0.41
1:A:388:LEU:HD12	1:A:388:LEU:HA	1.83	0.41
1:B:194:LYS:HD2	1:B:346:HIS:CE1	2.56	0.41
1:B:287:VAL:O	1:B:290:ALA:HB3	2.20	0.41
2:D:83:SER:HB3	2:D:86:SER:HB3	2.03	0.41
1:A:490:GLU:O	1:A:493:LYS:HB3	2.21	0.40
1:B:418:SER:O	1:B:419:LYS:C	2.58	0.40
1:B:519:GLN:O	1:B:520:MET:C	2.58	0.40
1:A:309:GLU:O	1:A:310:GLU:C	2.59	0.40
1:A:190:THR:HG22	1:A:191:GLU:N	2.35	0.40
1:A:348:GLN:HG3	1:A:349:GLU:HG3	2.02	0.40
1:B:404:LYS:HE2	1:B:428:ASP:OD1	2.21	0.40
1:B:411:ILE:HD11	1:B:482:TYR:CD1	2.56	0.40
2:C:62:GLU:HA	2:C:68:ARG:HD2	2.03	0.40
1:A:384:THR:HG22	1:A:388:LEU:HD22	2.03	0.40
1:A:547:HIS:CG	1:A:547:HIS:O	2.74	0.40
1:A:549:CYS:HB2	1:A:551:ALA:H	1.86	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:LYS:O	2:C:133:LYS:CB	2.68	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	368/378 (97%)	341 (93%)	25 (7%)	2 (0%)	29	52
1	B	362/378 (96%)	332 (92%)	28 (8%)	2 (1%)	25	47
2	C	175/177 (99%)	159 (91%)	15 (9%)	1 (1%)	25	47
2	D	156/177 (88%)	132 (85%)	22 (14%)	2 (1%)	12	24
All	All	1061/1110 (96%)	964 (91%)	90 (8%)	7 (1%)	22	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	87	PRO
1	A	238	ILE
2	C	133	LYS
1	B	238	ILE
1	B	261	PRO
2	D	29	PRO
1	A	261	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	299/339 (88%)	260 (87%)	39 (13%)	4	7
1	B	296/339 (87%)	260 (88%)	36 (12%)	5	9
2	C	132/153 (86%)	123 (93%)	9 (7%)	16	32
2	D	119/153 (78%)	108 (91%)	11 (9%)	9	17
All	All	846/984 (86%)	751 (89%)	95 (11%)	6	10

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	MET
1	A	190	THR
1	A	200	ARG
1	A	203	GLN
1	A	213	LEU
1	A	233	ILE
1	A	240	ILE
1	A	253	GLU
1	A	279	VAL
1	A	282	ARG
1	A	289	SER
1	A	308	LEU
1	A	317	ASN
1	A	330	MET
1	A	341	GLN
1	A	347	THR
1	A	348	GLN
1	A	355	ASN
1	A	372	GLU
1	A	387	GLN
1	A	388	LEU
1	A	396	SER
1	A	404	LYS
1	A	409	LEU
1	A	412	THR
1	A	415	GLU
1	A	427	LEU
1	A	431	LEU
1	A	436	ARG
1	A	439	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	440	SER
1	A	443	LEU
1	A	449	LEU
1	A	480	GLN
1	A	491	LEU
1	A	494	LYS
1	A	504	SER
1	A	526	THR
1	A	537	ARG
1	B	191	GLU
1	B	213	LEU
1	B	234	GLU
1	B	242	ASP
1	B	248	THR
1	B	249	HIS
1	B	255	LYS
1	B	260	THR
1	B	278	LEU
1	B	312	SER
1	B	319	ARG
1	B	325	LEU
1	B	330	MET
1	B	334	LEU
1	B	338	LEU
1	B	358	LEU
1	B	385	ASN
1	B	388	LEU
1	B	391	GLU
1	B	396	SER
1	B	409	LEU
1	B	418	SER
1	B	420	MET
1	B	447	VAL
1	B	450	HIS
1	B	451	SER
1	B	454	VAL
1	B	487	LYS
1	B	491	LEU
1	B	504	SER
1	B	506	ILE
1	B	532	CYS
1	B	533	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	535	LEU
1	B	560	ARG
1	B	561	VAL
2	C	41	SER
2	C	52	ASN
2	C	122	ASP
2	C	126	ILE
2	C	130	LYS
2	C	134	LEU
2	C	143	LEU
2	C	162	GLN
2	C	165	LEU
2	D	4	ILE
2	D	11	ASP
2	D	16	LYS
2	D	18	CYS
2	D	25	THR
2	D	62	GLU
2	D	87	PRO
2	D	101	VAL
2	D	102	ARG
2	D	135	THR
2	D	165	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	GLN
1	A	377	ASN
1	A	382	GLN
1	A	387	GLN
1	A	498	GLN
1	A	510	ASN
1	A	514	ASN
1	B	219	HIS
1	B	316	ASN
2	C	39	ASN
2	C	74	GLN
2	C	141	GLN
2	D	141	GLN
2	D	162	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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 ⓘ

### 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	372/378 (98%)	-0.12	5 (1%) 77 73	20, 38, 61, 69	0
1	B	368/378 (97%)	-0.07	5 (1%) 75 71	20, 40, 59, 67	0
2	C	177/177 (100%)	0.22	17 (9%) 8 5	20, 37, 65, 67	0
2	D	164/177 (92%)	0.71	21 (12%) 3 2	37, 67, 92, 93	0
All	All	1081/1110 (97%)	0.08	48 (4%) 34 27	20, 41, 75, 93	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	30	GLY	6.7
2	D	50	PRO	5.7
2	D	51	VAL	5.0
2	C	51	VAL	4.8
2	D	28	PHE	4.6
2	C	28	PHE	4.6
2	C	29	PRO	4.2
2	D	29	PRO	4.1
2	D	43	ASN	4.0
2	D	161	THR	4.0
1	B	565	GLY	3.9
2	C	124	ASP	3.8
1	A	260	THR	3.6
2	C	125	THR	3.5
2	C	50	PRO	3.4
2	D	122	ASP	3.1
2	C	42	ALA	3.0
2	D	132	LYS	3.0
2	D	135	THR	2.9
2	D	134	LEU	2.9
2	D	52	ASN	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	13	ALA	2.7
2	C	26	ASN	2.7
2	C	123	LYS	2.7
2	D	136	PRO	2.6
2	D	133	LYS	2.6
2	C	163	ARG	2.6
2	C	31	GLU	2.5
2	D	42	ALA	2.5
2	D	85	VAL	2.5
2	D	120	ARG	2.5
1	B	464	ASN	2.5
1	A	431	LEU	2.4
1	A	189	MET	2.4
2	C	32	TYR	2.3
1	A	348	GLN	2.3
1	B	394	ASP	2.3
2	C	127	GLU	2.3
1	B	437	ARG	2.2
2	D	118	ASP	2.2
2	C	126	ILE	2.1
2	C	43	ASN	2.1
2	C	177	LEU	2.1
2	C	1	MET	2.1
1	B	566	GLY	2.1
2	D	8	VAL	2.1
2	D	117	LEU	2.0
1	A	449	LEU	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 carbohydrates 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	ZN	B	2	1/1	0.99	0.08	44,44,44,44	0
3	ZN	A	1	1/1	1.00	0.11	32,32,32,32	0
3	ZN	A	4	1/1	1.00	0.07	32,32,32,32	0
3	ZN	B	3	1/1	1.00	0.12	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.