



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:37 pm BST

PDB ID : 2QVE  
Title : Crystal Structure of SgTAM bound to mechanism based inhibitor  
Authors : Christianson, C.V.; Montavon, T.J.; Bruner, S.D.  
Deposited on : 2007-08-08  
Resolution : 2.00 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

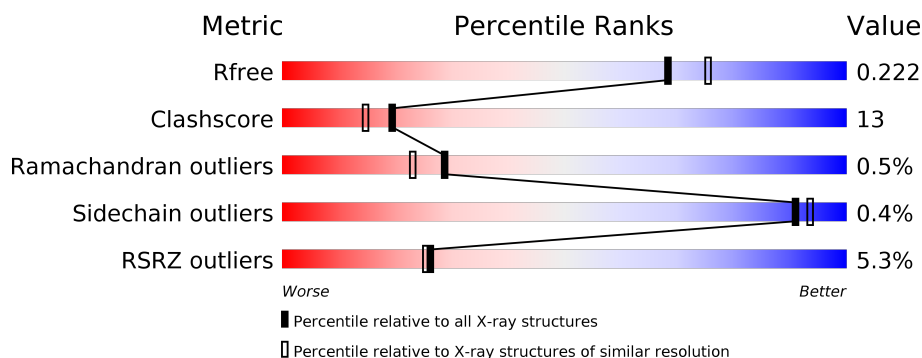
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	526	<div> <div>6%</div> <div>74%</div> <div>25%</div> </div>
1	B	526	<div> <div>5%</div> <div>80%</div> <div>20%</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	247	A	991	-	-	-	X
2	247	B	992	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8461 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.

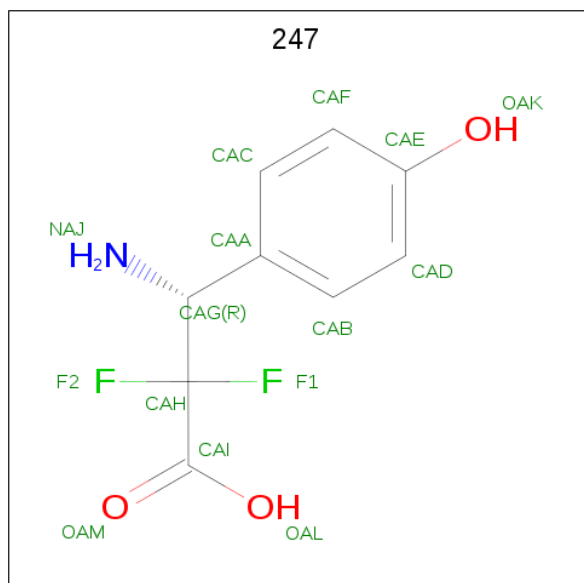
- Molecule 1 is a protein called Tyrosine Aminomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4007	2503	727	769	8			
1	B	526	Total	C	N	O	S	0	0	0
			4007	2503	727	769	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	MDO	ALA	CHROMOPHORE	UNP Q8GMG0
A	152	MDO	SER	CHROMOPHORE	UNP Q8GMG0
A	152	MDO	GLY	CHROMOPHORE	UNP Q8GMG0
B	152	MDO	ALA	CHROMOPHORE	UNP Q8GMG0
B	152	MDO	SER	CHROMOPHORE	UNP Q8GMG0
B	152	MDO	GLY	CHROMOPHORE	UNP Q8GMG0

- Molecule 2 is (3R)-3-amino-2,2-difluoro-3-(4-hydroxyphenyl)propanoic acid (three-letter code: 247) (formula: C<sub>9</sub>H<sub>9</sub>F<sub>2</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			15	9	2	1	3		
2	B	1	Total	C	F	N	O	0	0
			15	9	2	1	3		

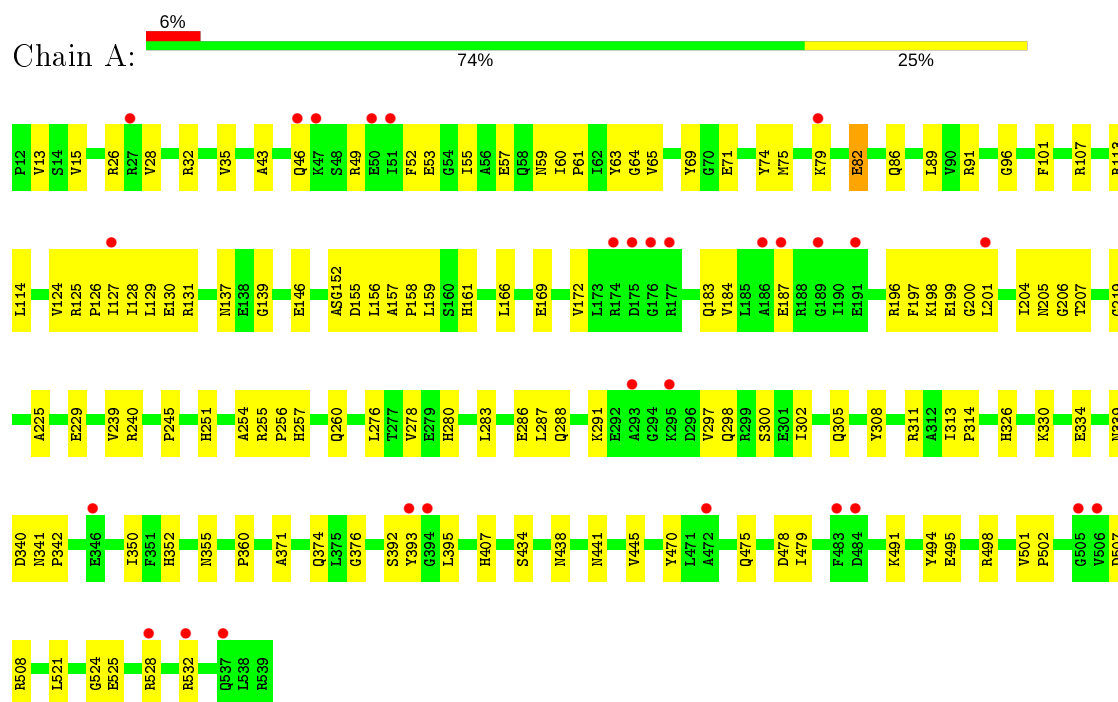
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	189	Total	O	0	0
			189	189		
3	B	228	Total	O	0	0
			228	228		

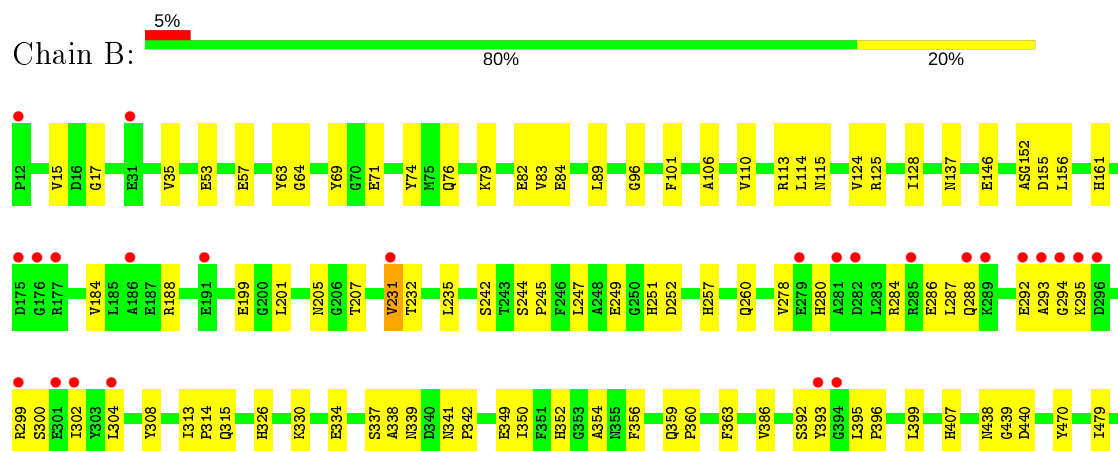
### 3 Residue-property plots [i](#)

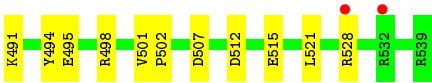
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Tyrosine Aminomutase



#### • Molecule 1: Tyrosine Aminomutase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.44Å 145.86Å 75.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (25.00-2.00) 93.5 (24.67-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.99Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.194 , 0.224 0.191 , 0.222	Depositor DCC
$R_{free}$ test set	6979 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.58% 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: 247, MDO

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	0.45	7/4053 (0.2%)	0.57	0/5490
1	B	0.43	5/4053 (0.1%)	0.59	0/5490
All	All	0.44	12/8106 (0.1%)	0.58	0/10980

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	TYR	CD1-CE1	-10.63	1.23	1.39
1	A	63	TYR	CD1-CE1	-10.55	1.23	1.39
1	A	63	TYR	CD2-CE2	-10.09	1.24	1.39
1	B	63	TYR	CZ-OH	-7.77	1.24	1.37
1	A	63	TYR	CZ-OH	-7.47	1.25	1.37
1	A	63	TYR	CE2-CZ	-6.97	1.29	1.38
1	B	63	TYR	CD2-CE2	-6.80	1.29	1.39
1	A	63	TYR	C-O	-6.73	1.10	1.23
1	B	63	TYR	CE2-CZ	-6.40	1.30	1.38
1	A	63	TYR	CE1-CZ	-5.89	1.30	1.38
1	B	63	TYR	CG-CD2	-5.86	1.31	1.39
1	A	63	TYR	CG-CD2	-5.25	1.32	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4007	0	4033	122	0
1	B	4007	0	4034	108	0
2	A	15	0	5	1	0
2	B	15	0	5	3	0
3	A	189	0	0	6	0
3	B	228	0	0	7	0
All	All	8461	0	8077	207	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 13.

All (207) 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:235:LEU:HD11	1:B:386:VAL:HG11	1.41	1.03
1:A:35:VAL:H	1:A:137:ASN:HD21	1.13	0.96
1:B:96:GLY:H	1:B:161:HIS:HE1	1.13	0.95
1:A:32:ARG:HH12	1:A:139:GLY:HA2	1.30	0.95
1:B:35:VAL:H	1:B:137:ASN:HD21	1.09	0.95
1:B:152:MDO:HB21	2:B:992:247:F2	1.66	0.86
1:A:475:GLN:HE21	1:A:479:ILE:HD11	1.41	0.85
1:A:251:HIS:HD2	1:A:260:GLN:HE21	1.22	0.85
1:A:32:ARG:NH1	1:A:139:GLY:HA2	1.91	0.85
1:B:235:LEU:HD11	1:B:386:VAL:CG1	2.08	0.84
1:A:305:GLN:HE22	1:B:341:ASN:HD21	1.29	0.81
1:A:360:PRO:HB3	3:B:1128:HOH:O	1.82	0.78
1:A:207:THR:H	1:A:339:ASN:HD22	1.32	0.77
1:B:251:HIS:HD2	1:B:260:GLN:HE21	1.32	0.77
1:A:96:GLY:H	1:A:161:HIS:HE1	1.34	0.75
1:A:64:GLY:HA3	1:A:201:LEU:HD22	1.70	0.74
1:A:251:HIS:CD2	1:A:260:GLN:HE21	2.06	0.73
1:A:71:GLU:H	1:A:438:ASN:HD21	1.37	0.73
1:A:152:MDO:HB21	1:B:308:TYR:OH	1.92	0.70
1:A:125:ARG:HD3	1:A:199:GLU:OE2	1.91	0.70
1:B:231:VAL:HG22	1:B:470:TYR:CE1	2.26	0.70
1:A:152:MDO:HB21	2:A:991:247:F2	1.81	0.69
1:B:96:GLY:H	1:B:161:HIS:CE1	2.02	0.69
1:B:247:LEU:HB3	1:B:249:GLU:OE2	1.91	0.68
1:A:498:ARG:HE	1:A:498:ARG:HA	1.59	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:O	1:A:495:GLU:HG2	1.94	0.68
1:B:330:LYS:HA	1:B:330:LYS:HE2	1.75	0.68
1:A:126:PRO:O	1:A:130:GLU:HG3	1.94	0.68
1:B:15:VAL:HG13	1:B:115:ASN:HD22	1.58	0.68
1:A:407:HIS:HD2	1:A:507:ASP:H	1.42	0.67
1:B:294:GLY:O	1:B:295:LYS:HD2	1.95	0.67
1:B:71:GLU:H	1:B:438:ASN:HD21	1.42	0.67
1:B:152:MDO:O	1:B:156:LEU:N	2.28	0.66
1:B:326:HIS:HD2	3:B:1211:HOH:O	1.80	0.65
1:A:172:VAL:HG21	1:A:184:VAL:HG21	1.77	0.64
1:A:308:TYR:OH	1:B:152:MDO:HB21	1.97	0.64
1:B:152:MDO:CB2	2:B:992:247:F2	2.35	0.64
1:B:251:HIS:CD2	1:B:260:GLN:HE21	2.14	0.64
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.79	0.63
1:A:91:ARG:HD3	1:A:169:GLU:OE1	1.98	0.63
1:B:286:GLU:HG2	1:B:302:ILE:HD13	1.80	0.63
1:B:184:VAL:O	1:B:188:ARG:HG3	1.99	0.62
1:B:53:GLU:O	1:B:57:GLU:HG2	1.99	0.62
1:B:124:VAL:HG13	1:B:128:ILE:HD12	1.80	0.62
1:B:287:LEU:HD21	1:B:302:ILE:HB	1.83	0.61
1:A:287:LEU:HD13	1:A:302:ILE:HB	1.82	0.60
1:A:86:GLN:HE21	1:A:200:GLY:H	1.49	0.59
1:A:239:VAL:HG12	1:A:239:VAL:O	2.03	0.59
1:A:69:TYR:CE2	1:A:89:LEU:HD22	2.36	0.59
1:B:491:LYS:O	1:B:495:GLU:HG3	2.02	0.58
1:B:17:GLY:H	1:B:115:ASN:ND2	2.00	0.58
1:B:284:ARG:HH21	1:B:288:GLN:HE22	1.51	0.58
1:A:183:GLN:O	1:A:187:GLU:HG3	2.03	0.58
1:B:71:GLU:H	1:B:438:ASN:ND2	2.01	0.58
1:B:407:HIS:HD2	1:B:507:ASP:H	1.52	0.57
1:A:239:VAL:HG13	1:A:393:TYR:HB3	1.87	0.57
1:A:127:ILE:HD12	1:A:128:ILE:N	2.19	0.57
1:A:438:ASN:HD22	1:A:441:ASN:HB3	1.69	0.57
1:B:128:ILE:HD11	1:B:199:GLU:HB3	1.86	0.57
1:B:235:LEU:CD1	1:B:386:VAL:HG11	2.26	0.57
1:A:207:THR:H	1:A:339:ASN:ND2	1.99	0.57
1:A:355:ASN:ND2	1:B:315:GLN:HE21	2.03	0.57
1:A:355:ASN:HD22	1:B:315:GLN:HE21	1.51	0.56
1:B:286:GLU:HG2	1:B:302:ILE:CD1	2.35	0.56
1:B:494:TYR:CE2	1:B:498:ARG:HG3	2.40	0.56
1:A:172:VAL:CG2	1:A:184:VAL:HG21	2.35	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:NE2	1:A:200:GLY:H	2.03	0.56
1:B:124:VAL:CG1	1:B:128:ILE:HB	2.35	0.56
1:B:128:ILE:CD1	1:B:199:GLU:HB3	2.36	0.55
1:B:207:THR:H	1:B:339:ASN:HD22	1.52	0.55
1:B:247:LEU:HD23	3:B:1034:HOH:O	2.06	0.55
1:A:291:LYS:HB3	1:A:298:GLN:NE2	2.22	0.55
1:A:525:GLU:HA	1:A:528:ARG:HD2	1.88	0.55
1:A:158:PRO:HG3	3:A:1009:HOH:O	2.06	0.55
1:A:55:ILE:CG2	1:A:60:ILE:HD11	2.37	0.55
1:B:292:GLU:O	1:B:294:GLY:N	2.40	0.54
1:B:512:ASP:HB2	3:B:1208:HOH:O	2.07	0.54
1:A:124:VAL:CG1	1:A:128:ILE:HG13	2.37	0.54
1:B:205:ASN:OD1	2:B:992:247:NAJ	2.41	0.54
1:B:494:TYR:CZ	1:B:498:ARG:HG3	2.43	0.54
1:A:49:ARG:HH21	1:A:196:ARG:NH1	2.04	0.54
1:B:407:HIS:CD2	1:B:507:ASP:H	2.26	0.54
1:A:300:SER:O	1:B:74:TYR:HB2	2.08	0.54
1:B:84:GLU:HG3	3:B:1113:HOH:O	2.07	0.54
1:B:231:VAL:HG22	1:B:470:TYR:CZ	2.42	0.53
1:B:396:PRO:HG3	1:B:479:ILE:HG21	1.89	0.53
1:A:240:ARG:HH11	1:A:276:LEU:HD23	1.74	0.53
1:A:392:SER:HB2	1:A:395:LEU:HD12	1.89	0.53
1:A:69:TYR:CZ	1:A:89:LEU:HD22	2.44	0.52
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.90	0.52
1:A:225:ALA:O	1:A:229:GLU:HG3	2.10	0.52
1:A:96:GLY:H	1:A:161:HIS:CE1	2.22	0.52
1:A:152:MDO:O	1:A:156:LEU:N	2.38	0.52
1:A:278:VAL:HG11	1:A:283:LEU:HG	1.90	0.52
1:A:35:VAL:H	1:A:137:ASN:ND2	1.95	0.51
1:A:288:GLN:OE1	1:A:291:LYS:HE2	2.10	0.51
1:A:59:ASN:HD21	1:A:79:LYS:HG2	1.75	0.51
1:A:15:VAL:HG11	1:A:114:LEU:HG	1.93	0.51
1:B:15:VAL:HG11	1:B:114:LEU:HG	1.93	0.50
1:B:284:ARG:NH2	1:B:288:GLN:HE22	2.09	0.50
1:A:494:TYR:CE2	1:A:498:ARG:HG3	2.47	0.50
1:A:74:TYR:HB2	1:B:300:SER:O	2.11	0.50
1:A:43:ALA:HA	1:A:46:GLN:HG2	1.93	0.50
1:A:280:HIS:HD2	1:B:349:GLU:HG3	1.76	0.50
1:B:251:HIS:HD2	1:B:260:GLN:NE2	2.07	0.49
1:B:287:LEU:CD2	1:B:302:ILE:HB	2.42	0.49
1:B:313:ILE:HB	1:B:314:PRO:HD3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PRO:CG	1:B:479:ILE:HG21	2.42	0.49
1:A:254:ALA:HB1	1:B:338:ALA:HB3	1.94	0.49
1:B:528:ARG:NH2	3:B:1073:HOH:O	2.46	0.49
1:B:231:VAL:CG2	1:B:470:TYR:CE1	2.95	0.48
1:B:470:TYR:CE1	1:B:521:LEU:HD21	2.47	0.48
1:A:251:HIS:HD2	1:A:260:GLN:NE2	2.01	0.48
1:A:334:GLU:OE1	1:B:257:HIS:HE1	1.96	0.48
1:B:128:ILE:HD11	1:B:199:GLU:CD	2.34	0.48
1:B:439:GLY:O	1:B:440:ASP:HB2	2.14	0.48
3:A:1010:HOH:O	1:B:326:HIS:HE1	1.96	0.47
1:A:65:VAL:HG22	1:A:198:LYS:HB2	1.95	0.47
1:B:15:VAL:CG1	1:B:115:ASN:HD22	2.25	0.47
1:B:17:GLY:H	1:B:115:ASN:HD21	1.62	0.47
1:B:232:THR:HG21	1:B:313:ILE:HD13	1.95	0.47
1:A:245:PRO:CG	1:A:311:ARG:HG3	2.45	0.47
1:B:69:TYR:CZ	1:B:89:LEU:HD22	2.49	0.47
1:A:524:GLY:O	1:A:528:ARG:HG3	2.15	0.47
1:A:86:GLN:HE22	1:A:201:LEU:H	1.62	0.47
1:A:32:ARG:NH1	1:A:107:ARG:NH1	2.62	0.47
1:A:86:GLN:HE21	1:A:200:GLY:N	2.11	0.47
1:A:59:ASN:ND2	1:A:79:LYS:HG2	2.29	0.47
1:A:32:ARG:HH11	1:A:107:ARG:NH1	2.13	0.46
1:B:498:ARG:HE	1:B:498:ARG:HA	1.81	0.46
1:A:508:ARG:HD3	3:A:1025:HOH:O	2.14	0.46
1:B:399:LEU:O	1:B:479:ILE:HD11	2.15	0.46
1:A:371:ALA:HA	1:B:363:PHE:CZ	2.51	0.46
1:B:57:GLU:O	1:B:79:LYS:HE2	2.15	0.46
1:A:475:GLN:HE21	1:A:479:ILE:CD1	2.20	0.46
1:A:532:ARG:HB3	1:A:532:ARG:NH1	2.31	0.45
1:A:75:MET:SD	1:B:299:ARG:HG2	2.56	0.45
1:A:32:ARG:HD3	1:A:107:ARG:CZ	2.46	0.45
1:A:286:GLU:HG2	1:A:302:ILE:HD13	1.97	0.45
1:B:342:PRO:HB2	1:B:350:ILE:HG22	1.98	0.45
1:B:64:GLY:HA3	1:B:201:LEU:HD22	1.97	0.45
1:A:434:SER:HB3	1:A:445:VAL:O	2.17	0.45
1:A:113:ARG:NH1	1:A:206:GLY:HA3	2.32	0.45
1:B:354:ALA:HA	1:B:356:PHE:CE2	2.52	0.45
1:A:313:ILE:HB	1:A:314:PRO:HD3	1.99	0.45
1:A:71:GLU:N	1:A:438:ASN:HD21	2.09	0.45
1:B:392:SER:HB2	1:B:395:LEU:HB2	1.99	0.45
1:B:249:GLU:H	1:B:249:GLU:CD	2.19	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HG3	1:A:166:LEU:HD22	1.98	0.44
1:A:297:VAL:HG23	1:A:297:VAL:O	2.17	0.44
1:A:352:HIS:CE1	1:B:280:HIS:NE2	2.86	0.44
1:A:159:LEU:HB3	1:A:204:ILE:HA	1.99	0.44
1:A:326:HIS:HE1	3:B:1085:HOH:O	2.00	0.44
1:B:515:GLU:OE1	1:B:515:GLU:HA	2.17	0.44
1:B:287:LEU:HD12	1:B:304:LEU:HD13	2.00	0.44
1:A:288:GLN:NE2	3:A:1087:HOH:O	2.50	0.44
1:A:374:GLN:OE1	1:A:374:GLN:HA	2.18	0.44
1:A:52:PHE:HZ	1:A:65:VAL:HG21	1.82	0.44
1:B:244:SER:N	1:B:245:PRO:CD	2.81	0.43
1:A:61:PRO:HD2	1:B:288:GLN:HG3	1.99	0.43
1:A:198:LYS:HG2	1:A:198:LYS:O	2.18	0.43
1:A:494:TYR:CZ	1:A:498:ARG:HG3	2.54	0.43
1:A:501:VAL:HA	1:A:502:PRO:HD3	1.84	0.43
1:B:124:VAL:HG12	1:B:125:ARG:O	2.18	0.43
1:A:342:PRO:HB2	1:A:350:ILE:HG22	2.00	0.43
1:A:71:GLU:H	1:A:438:ASN:ND2	2.09	0.43
1:A:291:LYS:HD2	1:B:76:GLN:HB3	1.99	0.43
1:B:242:SER:HA	1:B:278:VAL:O	2.19	0.43
1:A:158:PRO:HG3	3:A:1061:HOH:O	2.19	0.43
1:B:244:SER:HB2	1:B:280:HIS:HB2	2.01	0.43
1:A:113:ARG:HD2	1:A:113:ARG:HA	1.90	0.42
1:A:79:LYS:HB2	1:A:197:PHE:HZ	1.84	0.42
1:A:330:LYS:HZ3	1:B:257:HIS:HD2	1.66	0.42
1:B:284:ARG:HH21	1:B:288:GLN:NE2	2.16	0.42
1:A:61:PRO:CD	1:B:288:GLN:HG3	2.48	0.42
1:A:205:ASN:O	1:A:340:ASP:HA	2.18	0.42
1:A:86:GLN:NE2	1:A:200:GLY:N	2.66	0.42
1:A:305:GLN:HE22	1:B:341:ASN:ND2	2.08	0.42
1:A:257:HIS:HE1	1:B:334:GLU:OE1	2.02	0.42
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.19	0.42
1:A:101:PHE:CE2	1:A:146:GLU:HG2	2.55	0.42
1:A:470:TYR:CE1	1:A:521:LEU:HD21	2.55	0.42
1:B:232:THR:CG2	1:B:313:ILE:HD13	2.50	0.42
1:A:43:ALA:O	1:A:46:GLN:HG2	2.20	0.41
1:B:101:PHE:CE1	1:B:146:GLU:HA	2.55	0.41
1:B:205:ASN:HD21	1:B:341:ASN:HB3	1.84	0.41
1:B:359:GLN:N	1:B:360:PRO:HD2	2.35	0.41
1:A:131:ARG:HG3	1:A:166:LEU:CD2	2.50	0.41
1:A:341:ASN:OD1	1:A:342:PRO:HA	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:HH12	1:B:339:ASN:ND2	2.19	0.41
1:B:207:THR:H	1:B:339:ASN:ND2	2.18	0.41
1:A:35:VAL:N	1:A:137:ASN:HD21	1.97	0.41
1:B:106:ALA:O	1:B:110:VAL:HG23	2.20	0.41
1:B:69:TYR:CE2	1:B:89:LEU:HD22	2.56	0.41
1:A:26:ARG:HD2	1:A:219:GLY:HA3	2.03	0.41
1:A:255:ARG:HG3	1:B:337:SER:HB2	2.03	0.41
1:A:53:GLU:O	1:A:57:GLU:HG2	2.21	0.41
1:B:392:SER:O	1:B:393:TYR:HB2	2.21	0.41
1:B:501:VAL:HA	1:B:502:PRO:HD3	1.83	0.41
1:A:152:MDO:HB21	1:B:308:TYR:HH	1.84	0.41
1:A:308:TYR:HH	1:B:152:MDO:HB21	1.83	0.41
1:A:305:GLN:HE21	1:B:352:HIS:HB3	1.85	0.40
1:A:376:GLY:HA3	3:A:1032:HOH:O	2.21	0.40
1:A:82:GLU:OE2	1:A:196:ARG:HB3	2.21	0.40
1:A:129:LEU:HD12	1:A:129:LEU:N	2.36	0.40
1:A:13:VAL:HG21	1:A:28:VAL:HG23	2.02	0.40
1:B:82:GLU:HG2	1:B:83:VAL:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/526 (99%)	506 (97%)	14 (3%)	3 (1%)	25	19
1	B	523/526 (99%)	501 (96%)	20 (4%)	2 (0%)	34	30
All	All	1046/1052 (99%)	1007 (96%)	34 (3%)	5 (0%)	29	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	B	293	ALA
1	B	155	ASP
1	A	155	ASP
1	A	256	PRO

### 5.3.2 Protein sidechains ⓘ

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	415/415 (100%)	414 (100%)	1 (0%)	93	95
1	B	415/415 (100%)	413 (100%)	2 (0%)	88	92
All	All	830/830 (100%)	827 (100%)	3 (0%)	91	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	ASP
1	B	231	VAL
1	B	252	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	86	GLN
1	A	121	HIS
1	A	134	GLN
1	A	137	ASN
1	A	161	HIS
1	A	205	ASN
1	A	227	GLN
1	A	251	HIS
1	A	257	HIS
1	A	305	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	326	HIS
1	A	339	ASN
1	A	355	ASN
1	A	407	HIS
1	A	438	ASN
1	A	442	GLN
1	B	115	ASN
1	B	121	HIS
1	B	137	ASN
1	B	161	HIS
1	B	183	GLN
1	B	227	GLN
1	B	251	HIS
1	B	257	HIS
1	B	288	GLN
1	B	326	HIS
1	B	339	ASN
1	B	407	HIS
1	B	438	ASN
1	B	442	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MDO	A	152	1,2	12,13,14	2.44	4 (33%)	15,18,20	2.55	2 (13%)
1	MDO	B	152	1,2	12,13,14	2.42	4 (33%)	15,18,20	2.77	2 (13%)

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
1	MDO	A	152	1,2	-	2/4/23/24	0/1/1/1
1	MDO	B	152	1,2	-	1/4/23/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	MDO	O2-C2	6.37	1.36	1.23
1	B	152	MDO	O2-C2	6.31	1.36	1.23
1	A	152	MDO	CA2-N2	-2.98	1.33	1.39
1	B	152	MDO	CA2-N2	-2.96	1.33	1.39
1	A	152	MDO	C2-N3	-2.84	1.33	1.39
1	B	152	MDO	C2-N3	-2.82	1.33	1.39
1	A	152	MDO	C1-N3	-2.11	1.33	1.37
1	B	152	MDO	C1-N3	-2.10	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MDO	O2-C2-CA2	-7.55	126.72	130.96
1	B	152	MDO	CA2-C2-N3	6.78	106.58	103.37
1	A	152	MDO	CA2-C2-N3	6.72	106.55	103.37
1	A	152	MDO	O2-C2-CA2	-6.55	127.28	130.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152	MDO	N2-C1-CA-CB
1	B	152	MDO	N2-C1-CA-CB
1	A	152	MDO	N3-C1-CA-CB

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	152	MDO	4	0
1	B	152	MDO	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	247	A	991	1	11,15,15	10.05	2 (18%)	13,22,22	0.72	0
2	247	B	992	1	11,15,15	10.06	2 (18%)	13,22,22	0.73	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	247	A	991	1	-	2/9/16/16	0/1/1/1
2	247	B	992	1	-	4/9/16/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	991	247	F2-CAH	-23.60	1.09	1.37
2	B	992	247	F2-CAH	-23.57	1.09	1.37
2	B	992	247	F1-CAH	-23.57	1.09	1.37
2	A	991	247	F1-CAH	-23.48	1.09	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	991	247	CAB-CAA-CAG-CAH
2	A	991	247	CAC-CAA-CAG-CAH
2	B	992	247	CAB-CAA-CAG-CAH
2	B	992	247	CAC-CAA-CAG-CAH
2	B	992	247	NAJ-CAG-CAH-F1
2	B	992	247	NAJ-CAG-CAH-F2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	991	247	1	0
2	B	992	247	3	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	525/526 (99%)	0.22	29 (5%) 25 24	16, 28, 49, 62	0
1	B	525/526 (99%)	0.10	27 (5%) 28 27	15, 26, 48, 76	0
All	All	1050/1052 (99%)	0.16	56 (5%) 26 25	15, 27, 49, 76	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	LYS	7.2
1	B	293	ALA	5.6
1	B	393	TYR	5.0
1	B	296	ASP	4.9
1	A	175	ASP	4.4
1	A	293	ALA	4.3
1	B	176	GLY	3.8
1	B	532	ARG	3.7
1	A	393	TYR	3.5
1	B	302	ILE	3.5
1	B	294	GLY	3.4
1	A	295	LYS	3.2
1	B	175	ASP	3.2
1	B	288	GLN	3.2
1	B	528	ARG	3.1
1	A	484	ASP	3.1
1	A	532	ARG	3.0
1	A	47	LYS	3.0
1	B	12	PRO	3.0
1	A	174	ARG	2.9
1	A	528	ARG	2.9
1	A	394	GLY	2.9
1	B	186	ALA	2.8
1	A	79	LYS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	285	ARG	2.8
1	B	292	GLU	2.7
1	A	46	GLN	2.7
1	A	506	VAL	2.7
1	A	127	ILE	2.7
1	A	186	ALA	2.7
1	A	177	ARG	2.7
1	B	394	GLY	2.6
1	B	177	ARG	2.6
1	B	191	GLU	2.6
1	B	301	GLU	2.6
1	A	346	GLU	2.6
1	B	31	GLU	2.4
1	A	189	GLY	2.4
1	A	537	GLN	2.4
1	A	191	GLU	2.4
1	B	281	ALA	2.3
1	B	231	VAL	2.3
1	A	50	GLU	2.2
1	B	304	LEU	2.2
1	A	505	GLY	2.2
1	B	289	LYS	2.2
1	A	27	ARG	2.2
1	A	51	ILE	2.1
1	A	176	GLY	2.1
1	A	201	LEU	2.1
1	A	472	ALA	2.1
1	A	187	GLU	2.1
1	B	282	ASP	2.1
1	B	299	ARG	2.1
1	B	279	GLU	2.0
1	A	483	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MDO	B	152	13/14	0.85	0.16	21,27,30,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MDO	A	152	13/14	0.90	0.14	22,27,31,31	0

### 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( $\text{\AA}^2$ )	Q<0.9
2	247	B	992	15/15	0.42	0.62	26,32,33,33	0
2	247	A	991	15/15	0.53	0.57	26,33,35,38	0

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

There are no such residues in this entry.