



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:28 AM GMT

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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

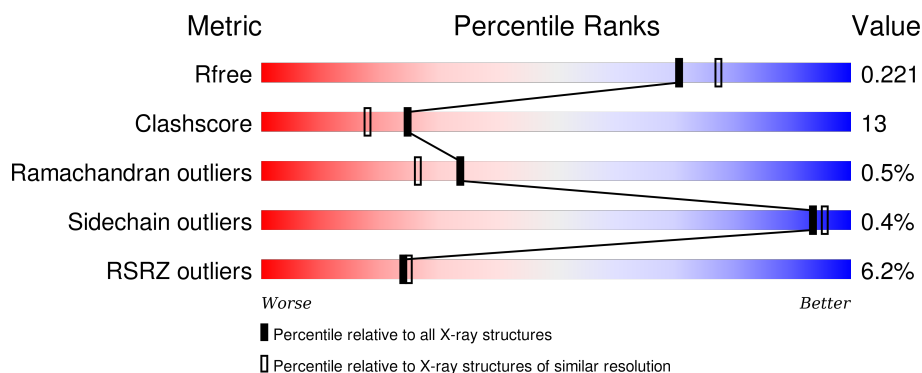
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

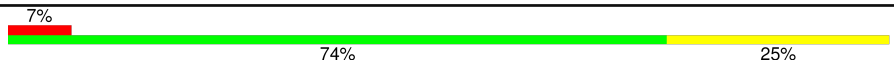

The reported resolution of this entry is 2.00 Å.

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	
1	B	526	

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



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.

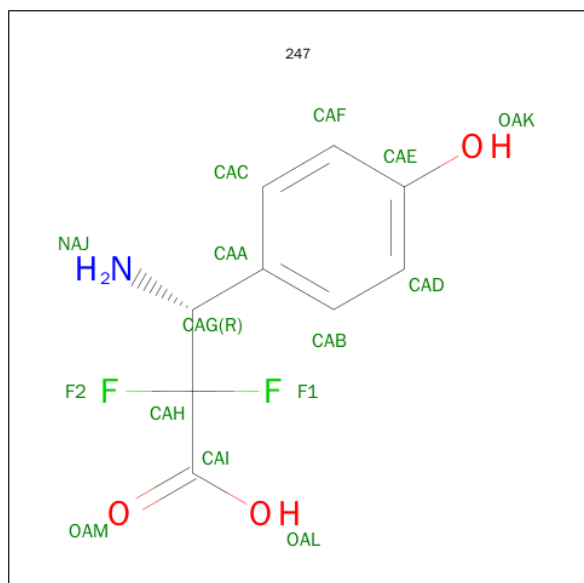
- Molecule 1 is a protein called Tyrosine Aminomutase.

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

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:  $C_9H_9F_2NO_3$ ).



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		

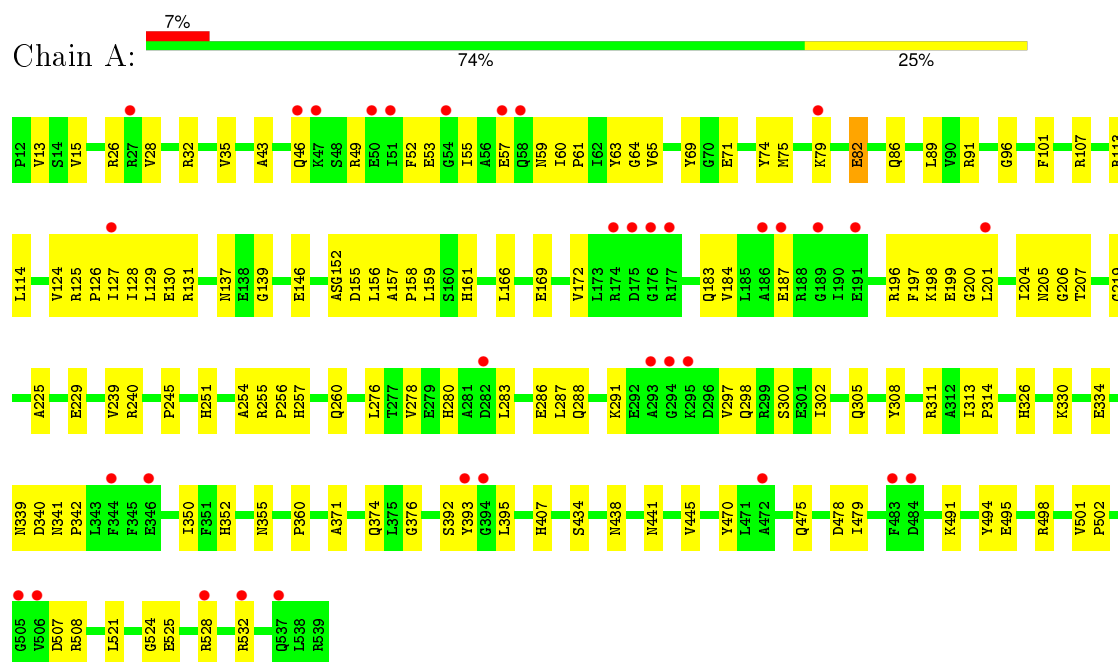
- Molecule 3 is water.

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 errors 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	Depositor
R, $R_{free}$	0.194 , 0.224 0.190 , 0.221	Depositor DCC
$R_{free}$ test set	6979 reflections (11.99%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 69021 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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:B:231:VAL:HG22	1:B:470:TYR:CE1	2.26	0.70
1:A:125:ARG:HD3	1:A:199:GLU:OE2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LYS:HA	1:B:330:LYS:HE2	1.75	0.68
1:A:491:LYS:O	1:A:495:GLU:HG2	1.94	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: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:A:330:LYS:HE2	1:A:330:LYS:HA	1.79	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:B:71:GLU:H	1:B:438:ASN:ND2	2.01	0.58
1:A:183:GLN:O	1:A:187:GLU:HG3	2.03	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

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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:525:GLU:HA	1:A:528:ARG:HD2	1.88	0.55
1:A:291:LYS:HB3	1:A:298:GLN:NE2	2.22	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:B:205:ASN:OD1	2:B:992:247:NAJ	2.41	0.54
1:A:124:VAL:CG1	1:A:128:ILE:HG13	2.37	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:96:GLY:H	1:A:161:HIS:CE1	2.22	0.52
1:A:225:ALA:O	1:A:229:GLU:HG3	2.10	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:280:HIS:HD2	1:B:349:GLU:HG3	1.76	0.50
1:A:43:ALA:HA	1:A:46:GLN:HG2	1.93	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:396:PRO:CG	1:B:479:ILE:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ILE:HB	1:B:314:PRO:HD3	1.94	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:B:69:TYR:CZ	1:B:89:LEU:HD22	2.49	0.47
1:A:245:PRO:CG	1:A:311:ARG:HG3	2.45	0.47
1:A:32:ARG:NH1	1:A:107:ARG:NH1	2.62	0.47
1:A:86:GLN:HE22	1:A:201:LEU:H	1.62	0.47
1:A:524:GLY:O	1:A:528:ARG:HG3	2.15	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:B:57:GLU:O	1:B:79:LYS:HE2	2.15	0.46
1:A:371:ALA:HA	1:B:363:PHE:CZ	2.51	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:64:GLY:HA3	1:B:201:LEU:HD22	1.97	0.45
1:B:342:PRO:HB2	1:B:350:ILE:HG22	1.98	0.45
1:A:434:SER:HB3	1:A:445:VAL:O	2.17	0.45
1:B:354:ALA:HA	1:B:356:PHE:CE2	2.52	0.45
1:A:113:ARG:NH1	1:A:206:GLY:HA3	2.32	0.45
1:A:71:GLU:N	1:A:438:ASN:HD21	2.09	0.45
1:A:313:ILE:HB	1:A:314:PRO:HD3	1.99	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

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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:326:HIS:HE1	3:B:1085:HOH:O	2.00	0.44
1:A:159:LEU:HB3	1:A:204:ILE:HA	1.99	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:52:PHE:HZ	1:A:65:VAL:HG21	1.82	0.44
1:A:374:GLN:OE1	1:A:374:GLN:HA	2.18	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:494:TYR:CZ	1:A:498:ARG:HG3	2.54	0.43
1:B:124:VAL:HG12	1:B:125:ARG:O	2.18	0.43
1:A:198:LYS:HG2	1:A:198:LYS:O	2.18	0.43
1:A:501:VAL:HA	1:A:502:PRO:HD3	1.84	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:A:342:PRO:HB2	1:A:350:ILE:HG22	2.00	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: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:79:LYS:HB2	1:A:197:PHE:HZ	1.84	0.42
1:A:113:ARG:HD2	1:A:113:ARG:HA	1.90	0.42
1:A:86:GLN:NE2	1:A:200:GLY:N	2.66	0.42
1:A:205:ASN:O	1:A:340:ASP:HA	2.18	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:B:232:THR:CG2	1:B:313:ILE:HD13	2.50	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: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:B:207:THR:H	1:B:339:ASN:ND2	2.18	0.41
1:B:113:ARG:HH12	1:B:339:ASN:ND2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:35:VAL:N	1:A:137:ASN:HD21	1.97	0.41
1:B:69:TYR:CE2	1:B:89:LEU:HD22	2.56	0.41
1:B:106:ALA:O	1:B:110:VAL:HG23	2.20	0.41
1:A:26:ARG:HD2	1:A:219:GLY:HA3	2.03	0.41
1:B:392:SER:O	1:B:393:TYR:HB2	2.21	0.41
1:A:53:GLU:O	1:A:57:GLU:HG2	2.21	0.41
1:A:255:ARG:HG3	1:B:337:SER:HB2	2.03	0.41
1:B:501:VAL:HA	1:B:502:PRO:HD3	1.83	0.41
1:A:308:TYR:HH	1:B:152:MDO:HB21	1.83	0.41
1:A:152:MDO:HB21	1:B:308:TYR:HH	1.84	0.41
1:A:305:GLN:HE21	1:B:352:HIS:HB3	1.85	0.40
1:A:82:GLU:OE2	1:A:196:ARG:HB3	2.21	0.40
1:A:376:GLY:HA3	3:A:1032:HOH:O	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%)	30	22
1	B	523/526 (99%)	501 (96%)	20 (4%)	2 (0%)	39	33
All	All	1046/1052 (99%)	1007 (96%)	34 (3%)	5 (0%)	34	26

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%)	95	97
1	B	415/415 (100%)	413 (100%)	2 (0%)	92	94
All	All	830/830 (100%)	827 (100%)	3 (0%)	93	95

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

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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	11,13,14	2.46	4 (36%)	13,18,20	2.65	2 (15%)
1	MDO	B	152	1,2	11,13,14	2.43	4 (36%)	13,18,20	2.90	2 (15%)



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	-	0/4/23/24	0/1/1/1
1	MDO	B	152	1,2	-	0/4/23/24	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	C2-N3	-3.10	1.33	1.39
1	B	152	MDO	C2-N3	-3.08	1.33	1.39
1	A	152	MDO	CA2-N2	-2.44	1.33	1.39
1	B	152	MDO	CA2-N2	-2.42	1.33	1.39
1	A	152	MDO	C1-N3	-2.10	1.33	1.37
1	B	152	MDO	C1-N3	-2.09	1.33	1.37
1	B	152	MDO	O2-C2	6.29	1.36	1.23
1	A	152	MDO	O2-C2	6.36	1.36	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MDO	O2-C2-CA2	-7.82	126.72	130.95
1	A	152	MDO	O2-C2-CA2	-6.79	127.28	130.95
1	A	152	MDO	CA2-C2-N3	6.05	106.55	103.39
1	B	152	MDO	CA2-C2-N3	6.10	106.58	103.39

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	10,15,15	9.80	2 (20%)	13,22,22	0.89	0
2	247	B	992	1	10,15,15	9.81	2 (20%)	13,22,22	0.91	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	-	0/8/16/16	0/1/1/1
2	247	B	992	1	-	0/8/16/16	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	-21.94	1.09	1.37
2	B	992	247	F2-CAH	-21.92	1.09	1.37
2	B	992	247	F1-CAH	-21.91	1.09	1.37
2	A	991	247	F1-CAH	-21.83	1.09	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	0.28	35 (6%) 21 22	16, 28, 49, 62	0
1	B	525/526 (99%)	0.16	30 (5%) 27 29	15, 26, 48, 76	0
All	All	1050/1052 (99%)	0.22	65 (6%) 24 25	15, 27, 49, 76	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	LYS	7.4
1	B	293	ALA	5.9
1	B	393	TYR	5.2
1	B	296	ASP	5.1
1	A	175	ASP	4.6
1	A	293	ALA	4.5
1	B	176	GLY	4.0
1	B	532	ARG	3.8
1	B	302	ILE	3.7
1	A	393	TYR	3.6
1	B	294	GLY	3.6
1	B	175	ASP	3.3
1	A	295	LYS	3.3
1	B	528	ARG	3.3
1	B	288	GLN	3.3
1	A	484	ASP	3.2
1	A	532	ARG	3.1
1	B	12	PRO	3.1
1	A	47	LYS	3.1
1	B	186	ALA	3.1
1	A	174	ARG	3.0
1	A	394	GLY	3.0
1	A	528	ARG	3.0
1	A	506	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	285	ARG	2.9
1	A	79	LYS	2.9
1	A	127	ILE	2.9
1	A	186	ALA	2.9
1	A	46	GLN	2.8
1	B	292	GLU	2.8
1	B	394	GLY	2.8
1	A	177	ARG	2.8
1	B	177	ARG	2.7
1	B	191	GLU	2.7
1	A	346	GLU	2.7
1	B	301	GLU	2.7
1	B	31	GLU	2.5
1	A	189	GLY	2.5
1	A	537	GLN	2.5
1	A	191	GLU	2.5
1	B	231	VAL	2.5
1	B	281	ALA	2.4
1	B	304	LEU	2.4
1	A	50	GLU	2.3
1	A	51	ILE	2.3
1	A	505	GLY	2.3
1	A	472	ALA	2.3
1	B	289	LYS	2.3
1	A	201	LEU	2.3
1	A	176	GLY	2.2
1	A	27	ARG	2.2
1	A	187	GLU	2.2
1	B	282	ASP	2.2
1	B	299	ARG	2.2
1	A	483	PHE	2.2
1	A	344	PHE	2.1
1	B	279	GLU	2.1
1	A	294	GLY	2.1
1	B	347	GLY	2.1
1	B	32	ARG	2.1
1	A	282	ASP	2.1
1	B	297	VAL	2.1
1	A	58	GLN	2.0
1	A	54	GLY	2.0
1	A	57	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MDO	A	152	13/14	0.90	0.14	-	22,27,31,31	0
1	MDO	B	152	13/14	0.85	0.16	-	21,27,30,31	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	247	B	992	15/15	0.42	0.62	24.47	26,32,33,33	0
2	247	A	991	15/15	0.53	0.57	13.99	26,33,35,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.