



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:23 PM UTC

PDB ID : 2QVE / pdb_00002qve
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

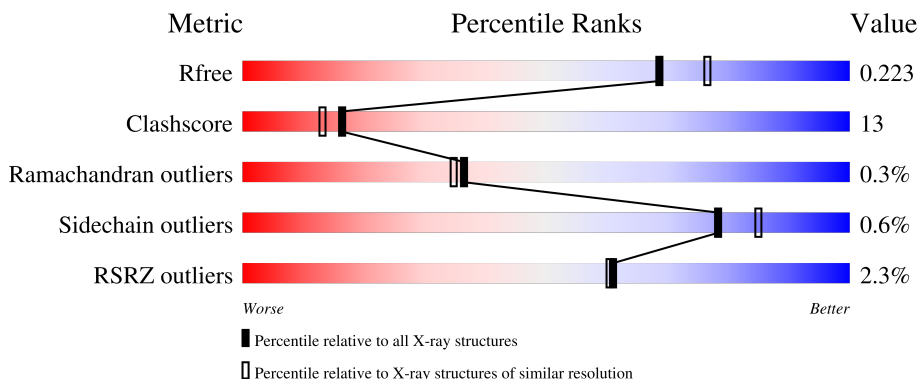
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	526	

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.

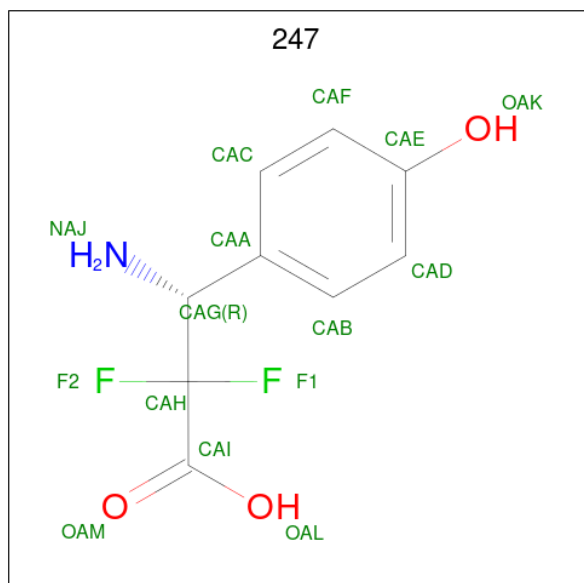
- Molecule 1 is a protein called Tyrosine Aminomutase.

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 (CCD ID: 247) (formula: C₉H₉F₂NO₃).



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		

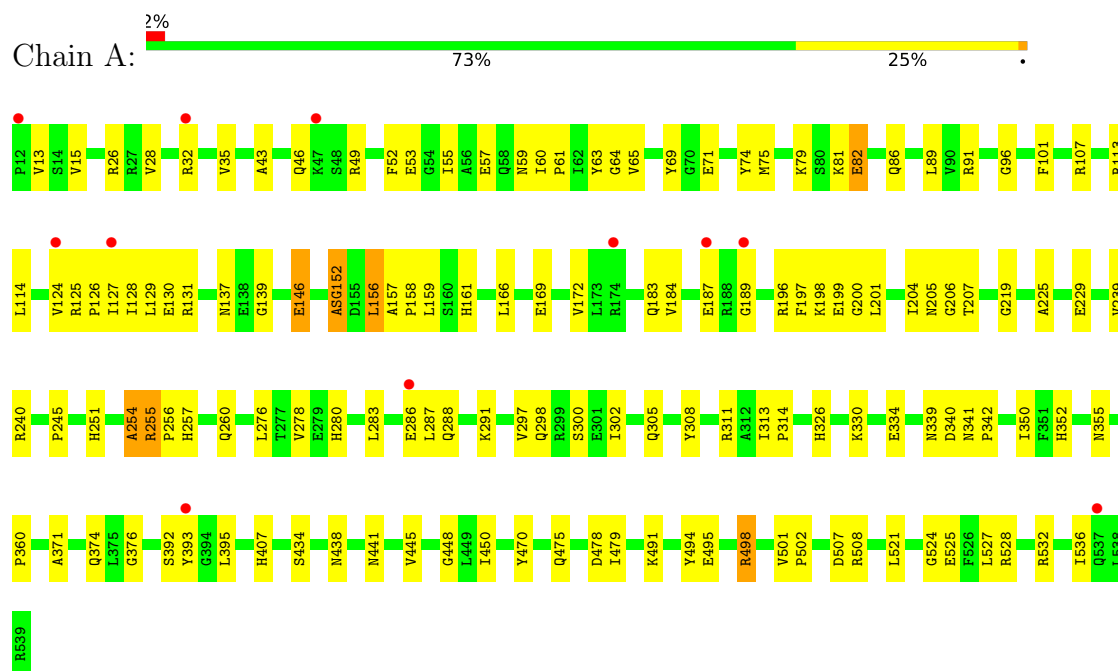
- Molecule 3 is water.

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

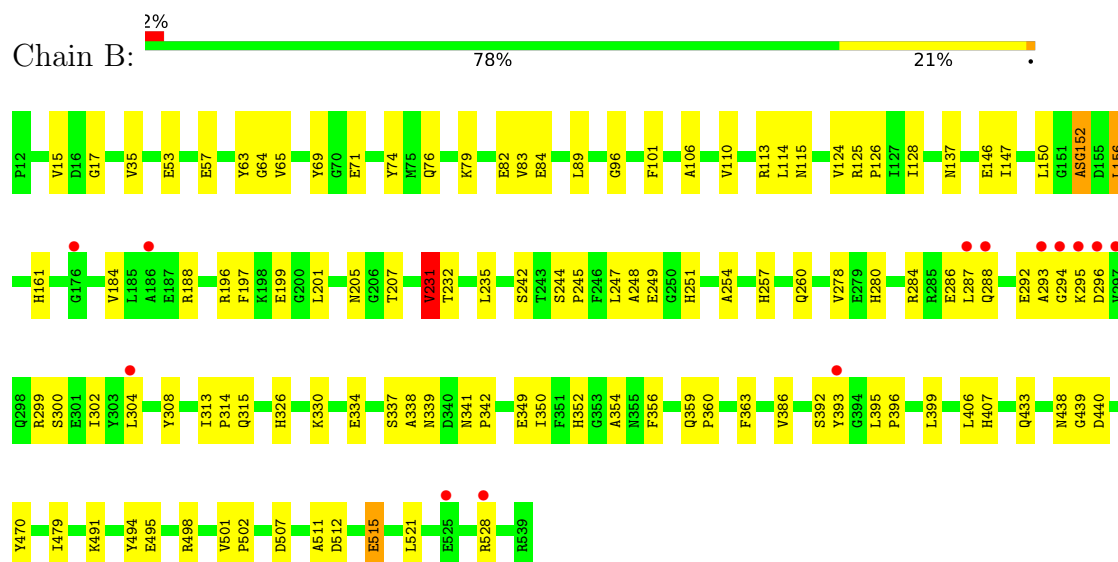
3 Residue-property plots

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: 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, α , β , γ	92.44Å 145.86Å 75.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (25.00-2.00) 93.4 (25.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 1.99Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.194 , 0.224 0.191 , 0.223	Depositor DCC
R_{free} test set	6979 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MDO, 247

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	0.46	3/4053 (0.1%)	0.90	10/5490 (0.2%)
1	B	0.44	3/4053 (0.1%)	0.92	11/5490 (0.2%)
All	All	0.45	6/8106 (0.1%)	0.91	21/10980 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	TYR	C-O	-10.90	1.10	1.23
1	B	63	TYR	CZ-OH	-6.38	1.24	1.38
1	A	63	TYR	CZ-OH	-6.14	1.25	1.38
1	B	63	TYR	C-O	-5.55	1.17	1.24
1	B	63	TYR	CD1-CE1	-5.08	1.23	1.38
1	A	63	TYR	CD1-CE1	-5.04	1.23	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	ASP	N-CA-C	7.83	119.60	111.14
1	A	255	ARG	CA-C-N	7.71	129.48	119.84
1	A	255	ARG	C-N-CA	7.71	129.48	119.84
1	B	231	VAL	CB-CA-C	-7.02	102.54	112.22
1	B	254	ALA	N-CA-C	7.01	118.57	111.07
1	B	156	LEU	N-CA-C	6.64	118.20	110.97
1	A	146	GLU	N-CA-C	6.53	119.39	111.82
1	A	254	ALA	N-CA-C	6.53	119.39	111.82
1	A	156	LEU	N-CA-C	6.38	118.81	111.02
1	A	448	GLY	N-CA-C	5.83	119.94	112.83
1	A	450	ILE	N-CA-C	-5.79	105.09	110.53
1	B	150	LEU	N-CA-C	-5.71	105.97	113.17
1	A	527	LEU	N-CA-C	-5.62	105.23	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	511	ALA	N-CA-C	5.58	118.09	111.33
1	B	147	ILE	N-CA-C	5.46	116.45	108.53
1	B	65	VAL	N-CA-C	-5.43	107.33	111.62
1	B	406	LEU	N-CA-C	-5.38	105.42	111.28
1	B	433	GLN	N-CA-C	5.34	118.63	112.97
1	A	536	ILE	N-CA-C	5.20	116.11	109.30
1	B	248	ALA	N-CA-C	5.15	117.56	111.33
1	A	189	GLY	N-CA-C	-5.06	108.27	115.30

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	4007	0	4026	124	0
1	B	4007	0	4026	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	8062	210	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 (210) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:498:ARG:HE	1.59	0.68
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:O3	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:A:330:LYS:HE2	1:A:330:LYS:HA	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:O	1:A:239:VAL:HG12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HD11	1:B:199:GLU:CD	2.34	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:O3	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:249:GLU:H	1:B:249:GLU:CD	2.19	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HH11	1:A:107:ARG:NH1	2.13	0.46
1:B:498:ARG:HA	1:B:498:ARG:HE	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:75:MET:SD	1:B:299:ARG:HG2	2.56	0.45
1:A:532:ARG:HB3	1:A:532:ARG:NH1	2.31	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: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: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: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:HA	1:B:515:GLU:OE1	2.17	0.44
1:B:287:LEU:HD12	1:B:304:LEU:HD13	2.00	0.44
1:A:52:PHE:HZ	1:A:65:VAL:HG21	1.82	0.44
1:A:196:ARG:O	1:A:197:PHE:C	2.60	0.44
1:A:288:GLN:NE2	3:A:1087:HOH:O	2.50	0.44
1:A:374:GLN:HA	1:A:374:GLN:OE1	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:198:LYS:O	1:A:198:LYS:HG2	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:81:LYS:O	1:A:82:GLU:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:A:113:ARG:HD2	1.90	0.42
1:B:284:ARG:HH21	1:B:288:GLN:NE2	2.16	0.42
1:A:86:GLN:NE2	1:A:200:GLY:N	2.66	0.42
1:A:127:ILE:HD12	1:A:127:ILE:C	2.44	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:B:196:ARG:O	1:B:197:PHE:C	2.63	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
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: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: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: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:308:TYR:HH	1:B:152:MDO:HB21	1.83	0.41
1:A:82:GLU:OE2	1:A:196:ARG:HB3	2.21	0.40
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:129:LEU:N	1:A:129:LEU:HD12	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
1:A:152:MDO:HB21	1:B:308:TYR:HH	1.85	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	521/526 (99%)	505 (97%)	14 (3%)	2 (0%)	30	27
1	B	521/526 (99%)	500 (96%)	20 (4%)	1 (0%)	43	42
All	All	1042/1052 (99%)	1005 (96%)	34 (3%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	B	293	ALA
1	A	256	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	415/415 (100%)	413 (100%)	2 (0%)	81	87
1	B	415/415 (100%)	412 (99%)	3 (1%)	76	82
All	All	830/830 (100%)	825 (99%)	5 (1%)	78	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	ASP
1	A	498	ARG
1	B	126	PRO

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Mol	Chain	Res	Type
1	B	231	VAL
1	B	515	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	227	GLN
1	A	251	HIS
1	A	257	HIS
1	A	305	GLN
1	A	326	HIS
1	A	339	ASN
1	A	355	ASN
1	A	384	ASN
1	A	407	HIS
1	A	414	GLN
1	A	438	ASN
1	A	441	ASN
1	A	442	GLN
1	A	475	GLN
1	B	115	ASN
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	2.60	4 (36%)	15,18,20	1.99	2 (13%)
1	MDO	B	152	1,2	11,13,14	2.58	4 (36%)	15,18,20	2.17	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	6.61	1.36	1.23
1	B	152	MDO	O2-C2	6.54	1.36	1.23
1	A	152	MDO	CA2-N2	-3.20	1.33	1.39
1	B	152	MDO	CA2-N2	-3.17	1.33	1.39
1	A	152	MDO	C2-N3	-2.97	1.33	1.40
1	B	152	MDO	C2-N3	-2.95	1.33	1.40
1	A	152	MDO	C1-N3	-2.23	1.33	1.37
1	B	152	MDO	C1-N3	-2.22	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	-6.74	126.72	131.02
1	A	152	MDO	O2-C2-CA2	-5.86	127.28	131.02
1	B	152	MDO	CA2-C2-N3	3.66	106.58	103.50
1	A	152	MDO	CA2-C2-N3	3.63	106.55	103.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152	MDO	N2-C1-CA1-CB
1	B	152	MDO	N2-C1-CA1-CB
1	A	152	MDO	N3-C1-CA1-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 oligosaccharides 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	14,15,15	5.80	2 (14%)	19,22,22	0.81	0
2	247	B	992	1	14,15,15	5.81	2 (14%)	19,22,22	0.83	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	-	3/14/16/16	0/1/1/1
2	247	B	992	1	-	7/14/16/16	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	-15.31	1.09	1.36
2	B	992	247	F2-CAH	-15.29	1.09	1.36
2	B	992	247	F1-CAH	-15.29	1.09	1.36
2	A	991	247	F1-CAH	-15.23	1.09	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (10) 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	A	991	247	CAG-CAH-CAI-OAM
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
2	B	992	247	CAG-CAH-CAI-OAM
2	B	992	247	CAC-CAA-CAG-NAJ
2	B	992	247	CAA-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, 95th 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 ²)	Q<0.9
1	A	525/526 (99%)	0.05	11 (2%) 63 63	16, 28, 49, 62	0
1	B	525/526 (99%)	-0.12	13 (2%) 58 58	15, 26, 48, 76	0
All	All	1050/1052 (99%)	-0.04	24 (2%) 61 60	15, 27, 49, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	ALA	4.5
1	B	393	TYR	3.8
1	A	47	LYS	3.6
1	B	295	LYS	3.3
1	B	186	ALA	3.3
1	B	288	GLN	3.1
1	B	294	GLY	3.0
1	B	296	ASP	2.9
1	B	287	LEU	2.8
1	A	187	GLU	2.8
1	A	393	TYR	2.8
1	B	304	LEU	2.5
1	A	12	PRO	2.5
1	A	124	VAL	2.4
1	A	32	ARG	2.4
1	B	297	VAL	2.3
1	A	537	GLN	2.3
1	A	174	ARG	2.2
1	A	286	GLU	2.2
1	B	176	GLY	2.2
1	B	528	ARG	2.1
1	B	525	GLU	2.1
1	A	127	ILE	2.1
1	A	189	GLY	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, 95th 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 ²)	Q<0.9
1	MDO	B	152	13/14	0.79	0.12	21,27,30,31	0
1	MDO	A	152	13/14	0.84	0.11	22,27,31,31	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
2	247	B	992	15/15	0.43	0.21	26,32,33,33	0
2	247	A	991	15/15	0.45	0.18	26,33,35,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.