



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:16 PM UTC

PDB ID : 4CSM / pdb_00004csm
Title : YEAST CHORISMATE MUTASE + TYR + ENDOOXABICYCLIC INHIBITOR
Authors : Straeter, N.; Schnappauf, G.; Braus, G.; Lipscomb, W.N.
Deposited on : 1997-07-14
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

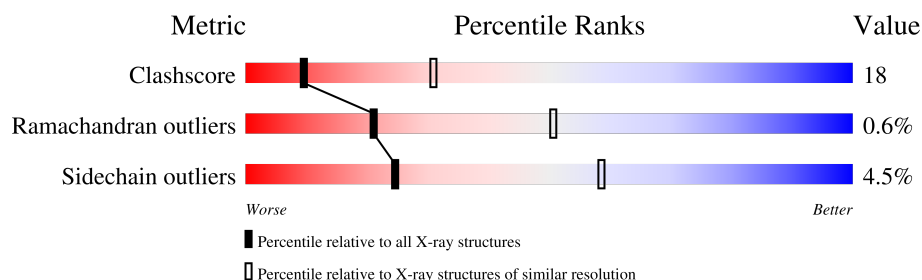
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	

2 Entry composition [i](#)

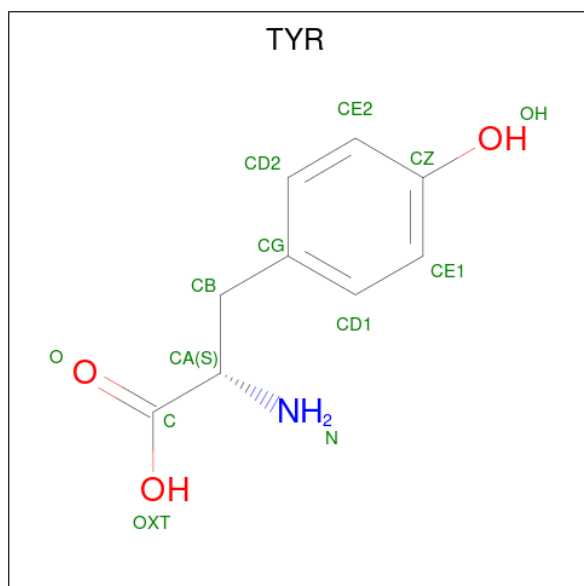
There are 3 unique types of molecules in this entry. The entry contains 4202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHORISMATE MUTASE.

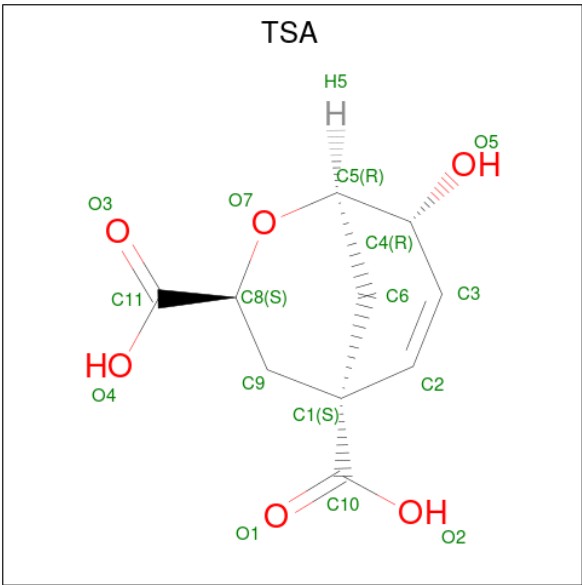
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2072	1335	346	386	5			
1	B	252	Total	C	N	O	S	0	0	0
			2072	1335	346	386	5			

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 3 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC ACID (CCD ID: TSA) (formula: $C_{10}H_{12}O_6$).



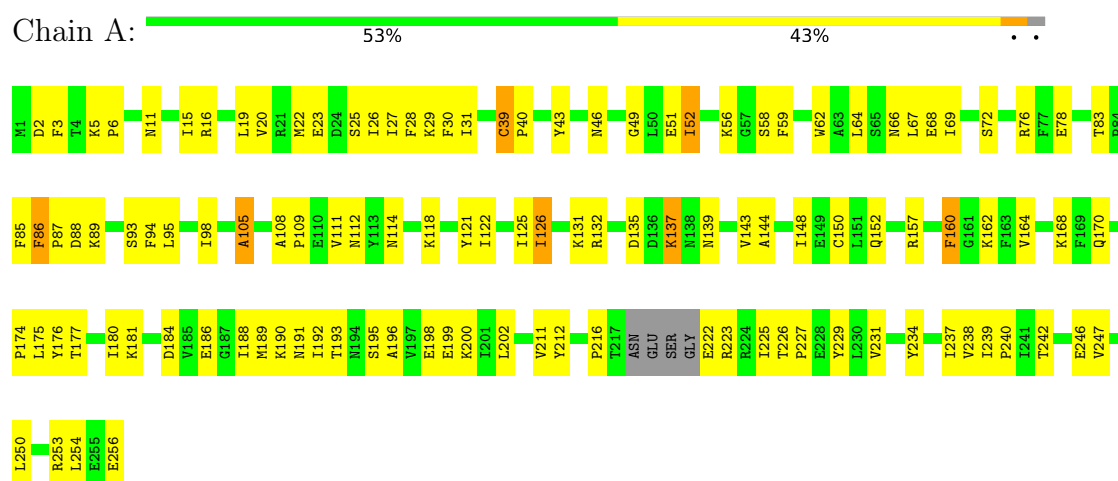
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		

3 Residue-property plots

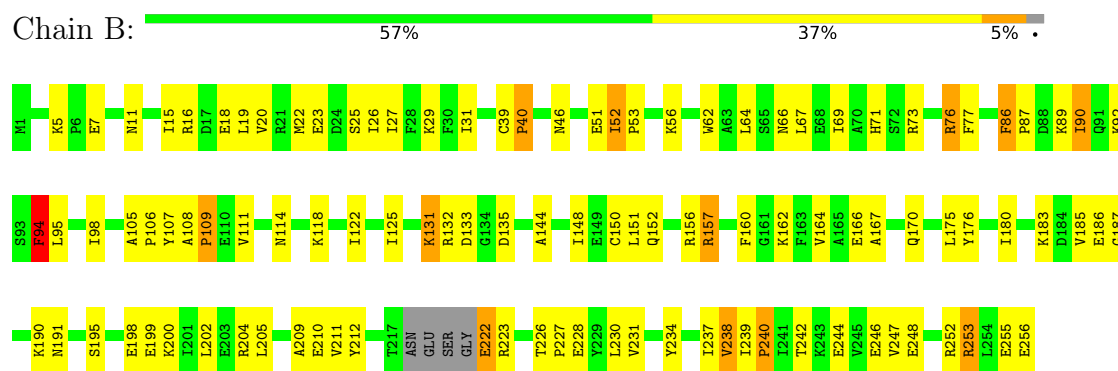
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	205.50Å 205.50Å 131.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.213 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4202	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.75	1/2116 (0.0%)	1.26	22/2857 (0.8%)
1	B	0.70	1/2116 (0.0%)	1.29	25/2857 (0.9%)
All	All	0.72	2/4232 (0.0%)	1.28	47/5714 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ILE	CA-CB	5.93	1.57	1.54
1	B	90	ILE	CA-CB	5.51	1.61	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	LYS	N-CA-C	8.44	120.17	110.97
1	B	125	ILE	N-CA-C	8.20	118.24	110.53
1	B	86	PHE	CA-C-N	8.09	128.55	119.32
1	B	86	PHE	C-N-CA	8.09	128.55	119.32
1	B	39	CYS	CA-C-N	7.95	127.51	119.24
1	B	39	CYS	C-N-CA	7.95	127.51	119.24
1	B	98	ILE	N-CA-C	-7.58	98.91	109.21
1	B	185	VAL	N-CA-C	7.24	117.32	110.30
1	A	86	PHE	CA-C-N	7.20	128.84	119.84
1	A	86	PHE	C-N-CA	7.20	128.84	119.84
1	A	105	ALA	CA-C-N	6.58	128.07	119.84
1	A	105	ALA	C-N-CA	6.58	128.07	119.84
1	B	94	PHE	N-CA-C	-6.56	95.92	107.73
1	B	238	VAL	N-CA-C	6.44	116.92	110.23
1	B	52	ILE	CA-C-N	6.40	127.84	119.84
1	B	52	ILE	C-N-CA	6.40	127.84	119.84
1	B	76	ARG	N-CA-C	6.36	117.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ILE	N-CA-C	-6.23	101.51	109.30
1	A	93	SER	N-CA-C	6.21	118.35	110.33
1	A	3	PHE	N-CA-C	6.16	120.52	113.19
1	A	125	ILE	N-CA-C	6.09	116.25	110.53
1	A	76	ARG	N-CA-C	5.95	117.45	110.97
1	A	112	ASN	N-CA-C	5.82	119.43	107.37
1	A	137	LYS	N-CA-C	5.80	123.16	110.80
1	A	39	CYS	CA-C-N	5.79	124.99	118.97
1	A	39	CYS	C-N-CA	5.79	124.99	118.97
1	A	52	ILE	CA-C-N	5.74	125.67	119.76
1	A	52	ILE	C-N-CA	5.74	125.67	119.76
1	B	105	ALA	CA-C-N	5.64	126.89	119.84
1	B	105	ALA	C-N-CA	5.64	126.89	119.84
1	A	83	THR	CA-C-N	5.57	125.47	119.85
1	A	83	THR	C-N-CA	5.57	125.47	119.85
1	A	78	GLU	N-CA-C	-5.51	106.52	113.18
1	B	89	LYS	N-CA-C	-5.50	106.15	112.92
1	A	250	LEU	N-CA-C	5.50	117.28	111.28
1	B	238	VAL	CA-C-N	5.41	123.65	120.24
1	B	238	VAL	C-N-CA	5.41	123.65	120.24
1	B	114	ASN	N-CA-C	5.38	117.90	111.71
1	A	49	GLY	N-CA-C	-5.33	108.35	114.69
1	B	253	ARG	N-CA-C	5.23	119.14	112.34
1	B	150	CYS	N-CA-C	-5.20	105.51	111.07
1	B	183	LYS	N-CA-C	-5.18	104.75	111.74
1	B	151	LEU	N-CA-C	5.16	117.30	111.11
1	B	77	PHE	N-CA-C	5.15	119.44	113.20
1	B	90	ILE	N-CA-C	5.11	116.32	108.71
1	A	150	CYS	N-CA-C	-5.01	104.91	111.02
1	A	181	LYS	N-CA-C	-5.00	105.72	111.07

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	2072	0	2107	79	0
1	B	2072	0	2107	72	0
2	A	13	0	8	0	0
2	B	13	0	8	1	0
3	A	16	0	10	0	0
3	B	16	0	10	2	0
All	All	4202	0	4250	150	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 18.

All (150) 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:202:LEU:HD12	1:B:231:VAL:HG13	1.44	0.96
1:A:202:LEU:HD12	1:A:231:VAL:HG13	1.50	0.94
1:A:19:LEU:HD22	1:A:157:ARG:HH11	1.36	0.88
1:B:94:PHE:HD1	1:B:94:PHE:H	1.31	0.77
1:B:25:SER:O	1:B:29:LYS:HD3	1.84	0.76
1:A:148:ILE:O	1:A:152:GLN:HG3	1.88	0.73
1:A:19:LEU:HD23	1:A:22:MET:HE3	1.70	0.73
1:A:66:ASN:O	1:A:69:ILE:HG12	1.89	0.72
1:B:94:PHE:CD1	1:B:94:PHE:N	2.58	0.71
1:B:23:GLU:O	1:B:27:ILE:HG13	1.90	0.71
1:B:157:ARG:HH21	1:B:238:VAL:HG12	1.55	0.71
1:B:157:ARG:O	1:B:160:PHE:HB2	1.90	0.70
1:A:157:ARG:O	1:A:160:PHE:HB2	1.92	0.70
1:A:202:LEU:HD12	1:A:231:VAL:CG1	2.20	0.70
1:B:175:LEU:HD21	1:B:191:ASN:HD21	1.57	0.70
1:A:22:MET:O	1:A:26:ILE:HG13	1.94	0.68
1:B:244:GLU:O	1:B:247:VAL:HG22	1.93	0.68
1:A:131:LYS:HG3	1:A:132:ARG:H	1.60	0.67
1:A:118:LYS:O	1:A:122:ILE:HG13	1.95	0.66
1:B:226:THR:HG22	1:B:228:GLU:H	1.60	0.66
1:A:144:ALA:O	1:A:148:ILE:HG13	1.98	0.64
1:B:27:ILE:O	1:B:31:ILE:HG12	1.98	0.64
1:A:16:ARG:O	1:A:20:VAL:HG23	1.98	0.64
1:A:27:ILE:O	1:A:31:ILE:HG12	1.98	0.63
1:A:237:ILE:C	1:A:240:PRO:HD2	2.24	0.63
1:A:223:ARG:HG3	1:B:228:GLU:OE2	1.98	0.62
1:A:64:LEU:O	1:A:68:GLU:HG3	1.99	0.61
1:A:157:ARG:NH2	1:A:234:TYR:HE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD21	1:A:191:ASN:HD21	1.66	0.61
1:B:19:LEU:HD22	1:B:157:ARG:HD3	1.81	0.61
1:A:186:GLU:O	1:A:190:LYS:HG2	2.01	0.61
1:B:73:ARG:HG2	1:B:94:PHE:HE1	1.66	0.61
1:B:148:ILE:O	1:B:152:GLN:HG3	2.02	0.60
1:A:227:PRO:O	1:A:231:VAL:HG23	2.02	0.59
1:B:66:ASN:O	1:B:69:ILE:HG12	2.02	0.59
1:B:52:ILE:HD13	1:B:62:TRP:CD2	2.38	0.59
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.83	0.59
1:A:46:ASN:HD21	1:A:56:LYS:HG2	1.68	0.58
1:A:52:ILE:HD13	1:A:62:TRP:CD2	2.39	0.58
1:A:198:GLU:O	1:A:202:LEU:HD23	2.03	0.58
1:B:94:PHE:O	1:B:95:LEU:HG	2.03	0.58
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.69	0.58
1:A:26:ILE:HG22	1:A:30:PHE:CE2	2.39	0.58
1:A:164:VAL:CG1	1:A:168:LYS:HE3	2.34	0.58
1:B:144:ALA:O	1:B:148:ILE:HG13	2.04	0.58
1:A:177:THR:HG23	1:A:254:LEU:HD11	1.85	0.57
1:A:176:TYR:O	1:A:180:ILE:HG13	2.05	0.57
1:B:186:GLU:O	1:B:190:LYS:HG2	2.04	0.56
1:B:247:VAL:HG23	1:B:248:GLU:N	2.20	0.55
1:B:11:ASN:O	1:B:15:ILE:HG13	2.07	0.54
1:B:107:TYR:HB2	1:B:252:ARG:NH2	2.22	0.54
1:B:205:LEU:HD22	1:B:230:LEU:HD21	1.89	0.54
1:A:11:ASN:O	1:A:15:ILE:HG13	2.06	0.54
1:A:19:LEU:HA	1:A:22:MET:HE3	1.89	0.54
1:A:164:VAL:HG12	1:A:168:LYS:HE3	1.90	0.54
1:B:73:ARG:HG2	1:B:94:PHE:CE1	2.43	0.54
1:A:25:SER:O	1:A:29:LYS:HD3	2.08	0.54
1:A:253:ARG:HH11	1:A:253:ARG:HG3	1.72	0.54
1:A:2:ASP:OD1	1:A:5:LYS:HG2	2.08	0.54
1:B:198:GLU:O	1:B:202:LEU:HD23	2.08	0.53
1:A:195:SER:O	1:A:199:GLU:HB2	2.09	0.53
1:B:67:LEU:CD2	1:B:148:ILE:HG21	2.39	0.53
1:B:40:PRO:HD2	1:B:135:ASP:OD1	2.08	0.53
1:B:252:ARG:O	1:B:255:GLU:HG3	2.07	0.53
1:A:67:LEU:CD2	1:A:148:ILE:HG21	2.39	0.53
1:A:121:TYR:CE2	1:A:126:ILE:HD11	2.44	0.53
1:A:69:ILE:O	1:A:72:SER:HB3	2.09	0.52
1:A:94:PHE:CD1	1:A:94:PHE:N	2.77	0.52
1:B:46:ASN:HD21	1:B:56:LYS:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:O	1:B:122:ILE:HG13	2.10	0.51
1:B:132:ARG:HG2	1:B:133:ASP:H	1.75	0.51
1:A:222:GLU:O	1:A:223:ARG:HB2	2.11	0.51
1:B:200:LYS:HE2	1:B:204:ARG:HH21	1.76	0.51
1:B:67:LEU:HD22	1:B:148:ILE:HG21	1.93	0.50
1:A:19:LEU:HD22	1:A:157:ARG:NH1	2.17	0.50
1:A:23:GLU:O	1:A:27:ILE:HG13	2.10	0.50
1:A:211:VAL:HG23	1:A:212:TYR:N	2.26	0.50
1:A:177:THR:HG23	1:A:254:LEU:CD1	2.42	0.50
1:A:31:ILE:HD13	1:A:225:ILE:HB	1.94	0.50
1:B:19:LEU:HD22	1:B:157:ARG:CD	2.41	0.50
1:A:28:PHE:O	1:A:31:ILE:HB	2.12	0.49
1:A:94:PHE:O	1:A:95:LEU:HG	2.12	0.49
1:A:242:THR:O	1:A:246:GLU:HG3	2.12	0.49
1:A:19:LEU:HD23	1:A:22:MET:CE	2.39	0.49
1:B:156:ARG:O	1:B:160:PHE:HD1	1.96	0.49
1:A:87:PRO:HG2	1:A:88:ASP:H	1.75	0.49
1:B:234:TYR:HA	1:B:238:VAL:HB	1.93	0.48
1:A:68:GLU:O	1:A:72:SER:HB2	2.13	0.48
1:B:19:LEU:HD23	1:B:22:MET:HE3	1.95	0.48
1:B:131:LYS:HG3	1:B:132:ARG:H	1.78	0.48
1:A:184:ASP:O	1:A:188:ILE:HG13	2.13	0.48
1:A:139:ASN:O	1:A:143:VAL:HG23	2.14	0.48
1:A:40:PRO:HD2	1:A:135:ASP:OD1	2.14	0.47
1:A:51:GLU:H	1:A:51:GLU:CD	2.22	0.47
1:B:16:ARG:O	1:B:20:VAL:HG23	2.13	0.47
1:A:118:LYS:HG2	1:A:122:ILE:HD11	1.97	0.47
1:B:211:VAL:HG23	1:B:212:TYR:N	2.30	0.47
1:B:111:VAL:HB	1:B:162:LYS:HE2	1.96	0.47
1:B:67:LEU:HD11	1:B:71:HIS:HE2	1.78	0.46
1:B:176:TYR:O	1:B:180:ILE:HG13	2.16	0.46
1:B:64:LEU:HG	1:B:86:PHE:HE1	1.81	0.46
1:B:166:GLU:O	1:B:170:GLN:HG2	2.16	0.46
1:A:189:MET:HE2	1:A:247:VAL:HG11	1.98	0.45
1:B:195:SER:O	1:B:199:GLU:HB2	2.16	0.45
1:A:234:TYR:HA	1:A:238:VAL:HB	1.98	0.45
1:A:237:ILE:O	1:A:240:PRO:HD2	2.17	0.45
1:B:222:GLU:O	1:B:223:ARG:HB2	2.16	0.45
1:B:164:VAL:HG11	3:B:400:TSA:H8	1.99	0.45
1:A:111:VAL:HB	1:A:162:LYS:HE2	1.99	0.45
1:A:170:GLN:HA	1:A:170:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HG23	3:B:400:TSA:O2	2.17	0.45
1:B:131:LYS:HG3	1:B:132:ARG:N	2.32	0.45
1:A:64:LEU:HD23	1:A:86:PHE:HE1	1.81	0.44
1:B:239:ILE:HB	1:B:240:PRO:HD3	2.00	0.44
1:A:39:CYS:O	1:A:43:TYR:CE2	2.71	0.44
1:B:5:LYS:HB3	1:B:7:GLU:OE2	2.18	0.43
1:B:76:ARG:HA	2:B:300:TYR:CD2	2.53	0.43
1:A:157:ARG:HE	1:A:238:VAL:CG1	2.32	0.43
1:A:192:ILE:HD12	1:A:193:THR:N	2.33	0.43
1:B:52:ILE:HD13	1:B:62:TRP:CE3	2.53	0.43
1:A:157:ARG:NH2	1:A:234:TYR:CE2	2.82	0.43
1:B:76:ARG:NH1	1:B:152:GLN:NE2	2.65	0.43
1:B:210:GLU:HA	1:B:223:ARG:HH22	1.83	0.43
1:B:92:LYS:HE3	1:B:92:LYS:HB2	1.88	0.43
1:B:187:GLY:O	1:B:191:ASN:HB2	2.19	0.43
1:B:195:SER:HA	1:B:198:GLU:HG2	2.00	0.43
1:B:211:VAL:HG23	1:B:212:TYR:CD1	2.54	0.43
1:A:196:ALA:O	1:A:200:LYS:HG3	2.18	0.42
1:A:39:CYS:N	1:A:40:PRO:HD3	2.34	0.42
1:B:237:ILE:C	1:B:240:PRO:HD2	2.45	0.42
1:B:242:THR:O	1:B:246:GLU:HG3	2.19	0.42
1:A:67:LEU:HD22	1:A:148:ILE:HG21	2.02	0.42
1:B:247:VAL:CG2	1:B:248:GLU:N	2.80	0.42
1:B:209:ALA:HB3	1:B:227:PRO:HG3	2.02	0.42
1:A:85:PHE:CD2	1:A:114:ASN:HB3	2.55	0.42
1:A:52:ILE:HD13	1:A:62:TRP:CG	2.55	0.41
1:A:174:PRO:HG2	1:A:175:LEU:H	1.84	0.41
1:A:58:SER:O	1:A:59:PHE:C	2.63	0.41
1:B:87:PRO:O	1:B:90:ILE:HG13	2.20	0.41
1:A:39:CYS:SG	1:A:143:VAL:HG21	2.61	0.41
1:A:226:THR:HB	1:A:229:TYR:CD2	2.55	0.41
1:B:18:GLU:O	1:B:22:MET:HG3	2.20	0.41
1:A:105:ALA:O	1:A:108:ALA:HB2	2.20	0.41
1:B:22:MET:O	1:B:26:ILE:HG13	2.20	0.41
1:A:239:ILE:N	1:A:240:PRO:CD	2.83	0.41
1:A:253:ARG:HG3	1:A:253:ARG:NH1	2.35	0.41
1:B:164:VAL:O	1:B:167:ALA:HB3	2.21	0.41
1:B:18:GLU:HG3	1:B:22:MET:HE2	2.03	0.40
1:A:67:LEU:HD23	1:A:148:ILE:HG21	2.03	0.40
1:A:108:ALA:HB3	1:A:109:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	248/256 (97%)	217 (88%)	28 (11%)	3 (1%)	10	34
1	B	248/256 (97%)	224 (90%)	24 (10%)	0	100	100
All	All	496/512 (97%)	441 (89%)	52 (10%)	3 (1%)	21	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LYS
1	A	137	LYS
1	A	216	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	50/237 (21%)	47 (94%)	3 (6%)	17	47
1	B	234/237 (99%)	224 (96%)	10 (4%)	26	60
All	All	284/474 (60%)	271 (95%)	13 (5%)	24	58

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	160	PHE
1	A	256	GLU

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Mol	Chain	Res	Type
1	B	40	PRO
1	B	51	GLU
1	B	53	PRO
1	B	94	PHE
1	B	106	PRO
1	B	109	PRO
1	B	157	ARG
1	B	222	GLU
1	B	240	PRO
1	B	256	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	13	GLN
1	B	102	GLN
1	B	152	GLN
1	B	191	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
3	TSA	A	400	-	16,17,17	1.55	3 (18%)	16,26,26	1.48	4 (25%)
3	TSA	B	400	-	16,17,17	1.33	2 (12%)	16,26,26	1.44	3 (18%)
2	TYR	A	300	-	12,13,13	0.84	0	13,17,17	0.31	0
2	TYR	B	300	-	12,13,13	1.21	1 (8%)	13,17,17	0.63	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
3	TSA	A	400	-	-	5/10/34/34	1/3/2/2
3	TSA	B	400	-	-	1/10/34/34	1/3/2/2
2	TYR	A	300	-	-	0/8/8/8	0/1/1/1
2	TYR	B	300	-	-	2/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	TSA	C3-C2	3.23	1.37	1.32
2	B	300	TYR	CE1-CD1	2.94	1.43	1.38
3	B	400	TSA	C3-C2	2.60	1.36	1.32
3	A	400	TSA	C9-C1	-2.55	1.51	1.55
3	B	400	TSA	O4-C11	-2.19	1.23	1.30
3	A	400	TSA	C8-C11	2.15	1.54	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	TSA	O7-C8-C9	3.17	114.45	109.95
3	B	400	TSA	C9-C8-C11	3.09	116.72	112.05
3	B	400	TSA	O4-C11-C8	2.90	120.24	112.71
3	A	400	TSA	C6-C1-C10	2.72	116.25	109.84
3	A	400	TSA	C9-C1-C10	-2.15	104.77	109.84
3	B	400	TSA	O5-C4-C5	2.08	115.35	110.94
3	A	400	TSA	O4-C11-C8	2.03	118.00	112.71

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	300	TYR	OXT-C-CA-N
3	A	400	TSA	C6-C1-C10-O2
3	A	400	TSA	C6-C1-C10-O1
2	B	300	TYR	O-C-CA-N
3	A	400	TSA	C2-C1-C10-O2
3	A	400	TSA	C9-C1-C10-O2
3	A	400	TSA	C2-C1-C10-O1
3	B	400	TSA	C9-C1-C10-O2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400	TSA	C1-C2-C3-C4-C5-C8-C9-O7
3	A	400	TSA	C1-C2-C3-C4-C5-C8-C9-O7

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	TSA	2	0
2	B	300	TYR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.