



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 05:34 AM EDT

PDB ID : 6I5Q  
Title : Papaver somniferum O-methyltransferase 1  
Authors : Cabry, M.P.; Offen, W.A.; Winzer, T.; Li, Y.; Graham, I.A.; Davies, G.J.; Saleh, P.  
Deposited on : 2018-11-14  
Resolution : 3.05 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 types of validation reports are described at

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

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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
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

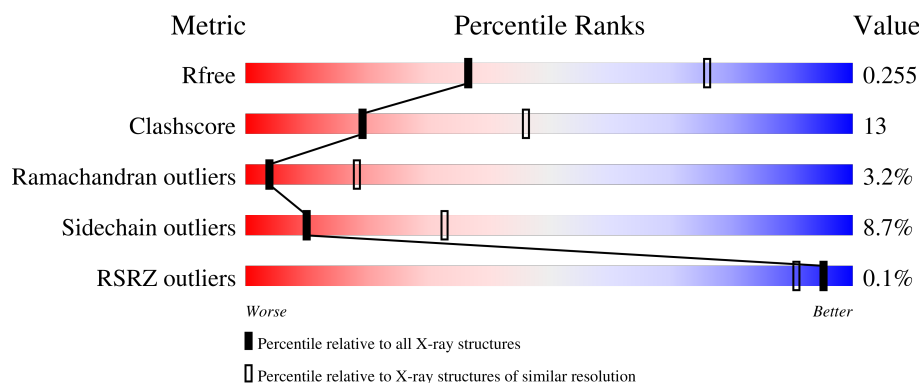
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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  $\geq 3$ , 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	393	<div> <div>60%</div> <div>24%</div> <div>•</div> <div>13%</div> </div>
1	B	393	<div> <div>56%</div> <div>28%</div> <div>•</div> <div>13%</div> </div>
1	C	393	<div> <div>66%</div> <div>20%</div> <div>•</div> <div>13%</div> </div>
1	D	393	<div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10068 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 O-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2546	1646	413	471	16			
1	B	342	Total	C	N	O	S	0	0	0
			2479	1588	407	467	17			
1	C	342	Total	C	N	O	S	0	0	0
			2512	1610	416	471	15			
1	D	346	Total	C	N	O	S	0	0	0
			2531	1616	421	478	16			

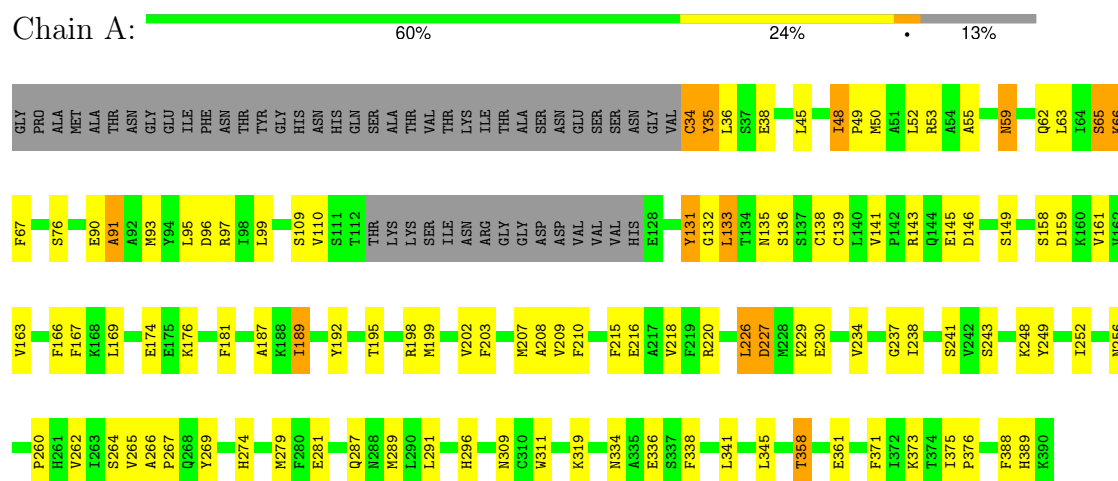
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP I3PLQ5
A	-1	PRO	-	expression tag	UNP I3PLQ5
A	0	ALA	-	expression tag	UNP I3PLQ5
B	-2	GLY	-	expression tag	UNP I3PLQ5
B	-1	PRO	-	expression tag	UNP I3PLQ5
B	0	ALA	-	expression tag	UNP I3PLQ5
C	-2	GLY	-	expression tag	UNP I3PLQ5
C	-1	PRO	-	expression tag	UNP I3PLQ5
C	0	ALA	-	expression tag	UNP I3PLQ5
D	-2	GLY	-	expression tag	UNP I3PLQ5
D	-1	PRO	-	expression tag	UNP I3PLQ5
D	0	ALA	-	expression tag	UNP I3PLQ5

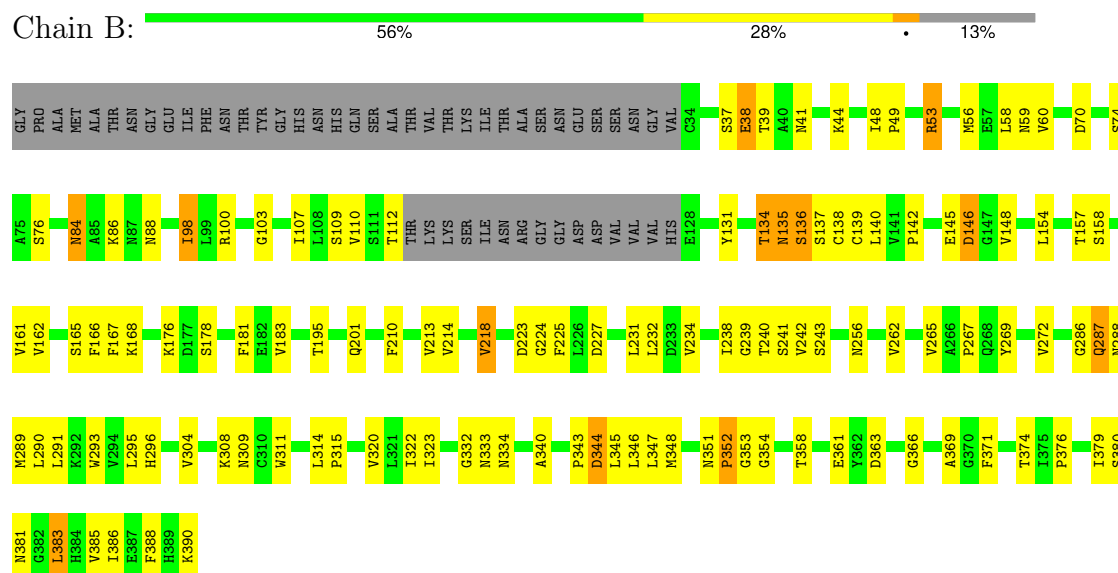
### 3 Residue-property plots

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: O-methyltransferase 1

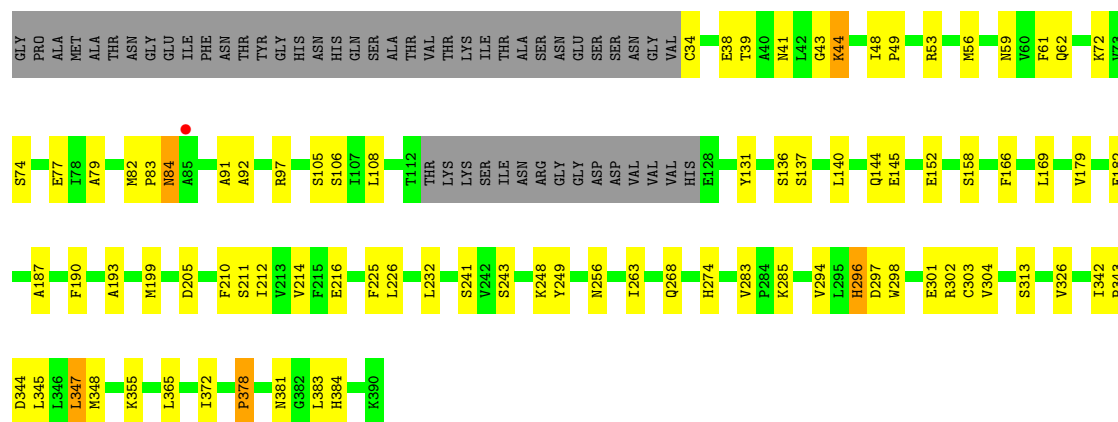


#### • Molecule 1: O-methyltransferase 1



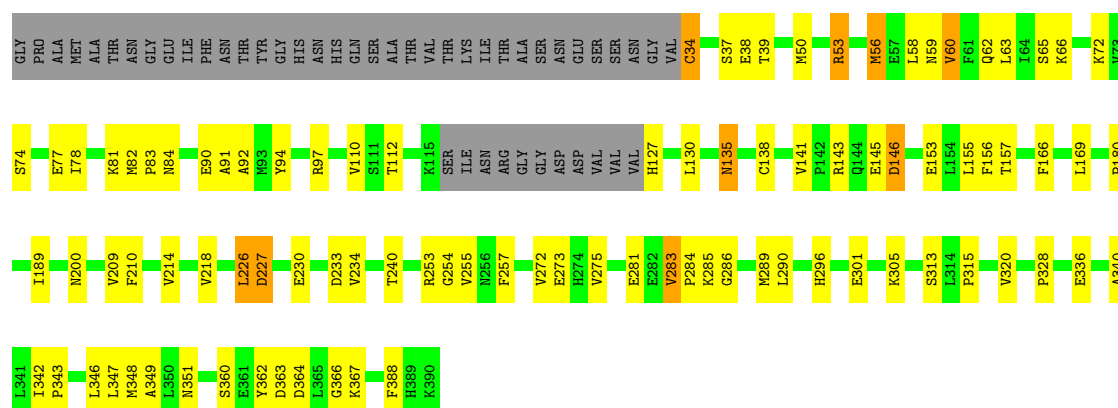
#### • Molecule 1: O-methyltransferase 1





● Molecule 1: O-methyltransferase 1

Chain D: 64% 21% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.00Å 112.00Å 304.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.00 – 3.05 97.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (97.00-3.05) 100.0 (97.00-3.05)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.210 , 0.256 0.215 , 0.255	Depositor DCC
$R_{free}$ test set	2067 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.6	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 92.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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](#)

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	0/2599	0.86	0/3533
1	B	0.77	0/2530	0.86	0/3440
1	C	0.76	0/2562	0.90	0/3483
1	D	0.80	0/2584	0.89	0/3513
All	All	0.77	0/10275	0.88	0/13969

There are no bond length outliers.

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	2546	0	2460	67	0
1	B	2479	0	2291	103	0
1	C	2512	0	2359	54	0
1	D	2531	0	2354	55	0
All	All	10068	0	9464	252	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 (252) 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:311:TRP:CD1	1:B:390:LYS:HE3	1.63	1.32
1:B:379:ILE:HD11	1:B:385:VAL:CG2	1.70	1.20
1:B:363:ASP:OD1	1:B:374:THR:OG1	1.69	1.09
1:B:379:ILE:CD1	1:B:385:VAL:HG23	1.83	1.08
1:B:379:ILE:HD11	1:B:385:VAL:HG23	1.10	1.05
1:A:358:THR:HG22	1:A:361:GLU:OE2	1.56	1.05
1:A:143:ARG:NH2	1:A:146:ASP:OD2	1.89	1.04
1:B:311:TRP:NE1	1:B:390:LYS:HE3	1.71	1.03
1:A:169:LEU:HD21	1:A:345:LEU:HD11	1.41	1.01
1:B:379:ILE:CD1	1:B:385:VAL:CG2	2.41	0.96
1:C:74:SER:CB	1:C:77:GLU:OE1	2.14	0.95
1:A:358:THR:CG2	1:A:361:GLU:OE2	2.14	0.94
1:C:144:GLN:HG2	1:C:145:GLU:OE1	1.68	0.93
1:A:96:ASP:OD1	1:A:131:TYR:OH	1.86	0.91
1:B:366:GLY:HA3	1:B:388:PHE:CE2	2.08	0.89
1:A:97:ARG:HH21	1:B:344:ASP:CG	1.78	0.85
1:C:97:ARG:HB3	1:D:348:MET:HE1	1.59	0.83
1:A:358:THR:CB	1:A:361:GLU:OE2	2.29	0.80
1:A:109:SER:O	1:A:131:TYR:HA	1.81	0.80
1:B:311:TRP:CD1	1:B:390:LYS:CE	2.57	0.79
1:B:311:TRP:NE1	1:B:390:LYS:CE	2.45	0.79
1:B:267:PRO:HG2	1:B:269:TYR:CZ	2.18	0.78
1:A:358:THR:HB	1:A:361:GLU:OE2	1.84	0.76
1:D:285:LYS:HA	1:D:313:SER:O	1.87	0.75
1:C:59:ASN:ND2	1:C:62:GLN:OE1	2.18	0.74
1:C:169:LEU:HD21	1:C:345:LEU:HD11	1.70	0.73
1:D:233:ASP:OD1	1:D:290:LEU:HD23	1.88	0.73
1:D:166:PHE:O	1:D:169:LEU:HB2	1.89	0.72
1:B:56:MET:CE	1:B:154:LEU:HD12	2.20	0.72
1:B:304:VAL:CG1	1:B:308:LYS:HE3	2.20	0.72
1:B:304:VAL:HG13	1:B:308:LYS:HE3	1.72	0.72
1:A:143:ARG:HH21	1:A:146:ASP:CG	1.92	0.71
1:B:379:ILE:HD11	1:B:385:VAL:HG21	1.69	0.70
1:D:340:ALA:O	1:D:343:PRO:HG2	1.92	0.70
1:B:56:MET:HE1	1:B:154:LEU:HD12	1.74	0.69
1:D:214:VAL:O	1:D:218:VAL:HG23	1.92	0.69
1:A:338:PHE:CD2	1:B:44:LYS:HD3	2.28	0.69
1:C:182:GLU:HG2	1:C:187:ALA:O	1.92	0.69
1:B:379:ILE:CG1	1:B:385:VAL:HG23	2.22	0.68
1:D:78:ILE:HG22	1:D:82:MET:HE3	1.76	0.68
1:C:97:ARG:CB	1:D:348:MET:HE1	2.23	0.67
1:A:48:ILE:HB	1:A:49:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:THR:HG23	1:B:137:SER:CB	2.25	0.67
1:B:311:TRP:HD1	1:B:390:LYS:HG3	1.60	0.67
1:A:338:PHE:CE2	1:B:44:LYS:HD2	2.30	0.66
1:B:358:THR:CB	1:B:361:GLU:OE1	2.43	0.66
1:B:157:THR:HG22	1:B:346:LEU:HD11	1.76	0.66
1:D:143:ARG:NH2	1:D:146:ASP:OD2	2.29	0.66
1:B:109:SER:O	1:B:131:TYR:HA	1.96	0.66
1:C:343:PRO:O	1:C:347:LEU:HB2	1.96	0.65
1:A:226:LEU:O	1:A:227:ASP:CB	2.44	0.65
1:B:311:TRP:CD1	1:B:390:LYS:HG3	2.31	0.65
1:B:379:ILE:CD1	1:B:385:VAL:HG21	2.23	0.65
1:C:344:ASP:OD1	1:D:97:ARG:NH2	2.27	0.65
1:D:328:PRO:HG3	1:D:336:GLU:HG2	1.79	0.65
1:A:198:ARG:O	1:A:202:VAL:HG23	1.96	0.64
1:A:34:CYS:O	1:A:34:CYS:SG	2.57	0.63
1:C:378:PRO:HA	1:C:384:HIS:CD2	2.32	0.63
1:A:237:GLY:HA2	1:A:262:VAL:HG11	1.81	0.62
1:C:256:ASN:HD22	1:C:274:HIS:CE1	2.17	0.62
1:B:320:VAL:CG1	1:B:388:PHE:HB2	2.29	0.62
1:D:78:ILE:HG22	1:D:82:MET:CE	2.29	0.62
1:C:378:PRO:HG3	1:C:384:HIS:HE2	1.64	0.61
1:A:95:LEU:CG	1:A:99:LEU:HD11	2.30	0.61
1:D:53:ARG:HG3	1:D:53:ARG:HH11	1.67	0.60
1:D:257:PHE:HD1	1:D:275:VAL:O	1.85	0.60
1:D:328:PRO:HG3	1:D:336:GLU:CG	2.31	0.60
1:B:332:GLY:C	1:B:334:ASN:H	2.05	0.59
1:D:257:PHE:HE2	1:D:283:VAL:HG23	1.67	0.59
1:A:176:LYS:HA	1:B:88:ASN:ND2	2.17	0.59
1:D:180:PRO:HG2	1:D:349:ALA:HA	1.84	0.59
1:C:59:ASN:OD1	1:C:62:GLN:HB3	2.03	0.59
1:B:231:LEU:HA	1:B:288:ASN:O	2.04	0.58
1:B:347:LEU:HD13	1:B:351:ASN:HB3	1.86	0.58
1:A:45:LEU:O	1:B:49:PRO:HG3	2.03	0.58
1:C:59:ASN:OD1	1:C:62:GLN:CB	2.52	0.58
1:A:238:ILE:HA	1:A:266:ALA:HB2	1.87	0.56
1:D:257:PHE:HA	1:D:275:VAL:O	2.05	0.56
1:B:168:LYS:HD2	1:B:183:VAL:HG12	1.86	0.56
1:A:136:SER:HA	1:B:38:GLU:HG3	1.87	0.56
1:A:38:GLU:CB	1:B:136:SER:OG	2.54	0.56
1:A:210:PHE:HE1	1:B:39:THR:HG21	1.70	0.56
1:A:199:MET:HE2	1:A:203:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ALA:O	1:B:343:PRO:HG2	2.05	0.55
1:C:263:ILE:HG23	1:C:274:HIS:HB3	1.89	0.55
1:C:48:ILE:N	1:C:49:PRO:HD2	2.22	0.55
1:A:159:ASP:OD2	1:A:161:VAL:HG13	2.06	0.55
1:D:60:VAL:O	1:D:63:LEU:N	2.38	0.55
1:C:39:THR:O	1:C:43:GLY:HA3	2.07	0.55
1:C:82:MET:O	1:C:84:ASN:N	2.40	0.55
1:B:84:ASN:OD1	1:B:84:ASN:N	2.40	0.55
1:B:134:THR:OG1	1:B:135:ASN:N	2.40	0.55
1:D:53:ARG:HH11	1:D:53:ARG:CG	2.19	0.55
1:C:97:ARG:HB3	1:D:348:MET:CE	2.35	0.55
1:C:166:PHE:HB3	1:D:50:MET:HB3	1.88	0.54
1:A:169:LEU:HG	1:B:98:ILE:HD13	1.89	0.54
1:D:257:PHE:CE2	1:D:283:VAL:HG23	2.43	0.54
1:A:163:VAL:O	1:A:166:PHE:N	2.41	0.53
1:B:56:MET:HE3	1:B:154:LEU:CD1	2.39	0.53
1:B:267:PRO:HG2	1:B:269:TYR:OH	2.08	0.53
1:B:295:LEU:HD11	1:B:322:ILE:HD13	1.91	0.53
1:B:320:VAL:HG12	1:B:388:PHE:HB2	1.90	0.53
1:B:320:VAL:HG13	1:B:320:VAL:O	2.09	0.53
1:C:342:ILE:HB	1:C:343:PRO:HD3	1.90	0.53
1:A:215:PHE:O	1:A:218:VAL:N	2.42	0.52
1:B:347:LEU:HD12	1:B:354:GLY:HA3	1.91	0.52
1:A:338:PHE:CE2	1:B:44:LYS:CD	2.92	0.52
1:B:286:GLY:O	1:B:314:LEU:HA	2.10	0.52
1:D:74:SER:H	1:D:77:GLU:HB2	1.75	0.52
1:A:319:LYS:HA	1:A:388:PHE:O	2.10	0.52
1:B:56:MET:CE	1:B:154:LEU:CD1	2.88	0.52
1:C:136:SER:CB	1:D:38:GLU:OE1	2.58	0.51
1:D:320:VAL:CG1	1:D:388:PHE:HB2	2.40	0.51
1:B:351:ASN:O	1:B:352:PRO:C	2.48	0.51
1:A:311:TRP:HB2	1:A:371:PHE:CE1	2.46	0.51
1:B:142:PRO:HA	1:B:148:VAL:O	2.11	0.51
1:B:347:LEU:O	1:B:351:ASN:O	2.29	0.51
1:A:136:SER:CB	1:B:38:GLU:OE2	2.59	0.50
1:A:338:PHE:CD2	1:B:44:LYS:CD	2.94	0.50
1:D:81:LYS:O	1:D:83:PRO:HD3	2.10	0.50
1:C:179:VAL:HB	1:C:182:GLU:HB2	1.92	0.50
1:D:135:ASN:O	1:D:138:CYS:HB2	2.11	0.50
1:D:230:GLU:HG3	1:D:253:ARG:HB3	1.93	0.50
1:A:93:MET:O	1:A:97:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLU:OE1	1:C:145:GLU:N	2.43	0.50
1:B:269:TYR:HB2	1:B:272:VAL:CB	2.42	0.50
1:C:79:ALA:HA	1:C:82:MET:HG3	1.94	0.50
1:B:181:PHE:CD1	1:B:181:PHE:C	2.86	0.49
1:D:320:VAL:HG12	1:D:388:PHE:HB2	1.94	0.49
1:B:146:ASP:OD1	1:B:146:ASP:N	2.46	0.49
1:A:230:GLU:HB3	1:A:287:GLN:HB2	1.94	0.49
1:A:199:MET:HE1	1:A:203:PHE:CE2	2.48	0.49
1:B:379:ILE:HG12	1:B:383:LEU:O	2.13	0.48
1:D:58:LEU:O	1:D:60:VAL:N	2.46	0.48
1:B:210:PHE:O	1:B:213:VAL:HG22	2.12	0.48
1:A:62:GLN:HA	1:A:141:VAL:HG13	1.96	0.48
1:D:34:CYS:O	1:D:37:SER:N	2.44	0.48
1:C:193:ALA:HA	1:C:199:MET:HE2	1.95	0.48
1:B:214:VAL:O	1:B:218:VAL:HG23	2.14	0.48
1:B:308:LYS:HG3	1:B:369:ALA:CB	2.44	0.48
1:D:56:MET:HE3	1:D:155:LEU:HG	1.96	0.48
1:C:48:ILE:HG12	1:C:105:SER:OG	2.14	0.47
1:C:225:PHE:O	1:C:226:LEU:C	2.51	0.47
1:C:82:MET:C	1:C:84:ASN:H	2.16	0.47
1:D:255:VAL:HA	1:D:273:GLU:O	2.13	0.47
1:D:53:ARG:CG	1:D:53:ARG:NH1	2.75	0.47
1:A:216:GLU:O	1:A:220:ARG:HG3	2.14	0.47
1:B:379:ILE:CG1	1:B:383:LEU:O	2.63	0.47
1:A:229:LYS:O	1:A:252:ILE:HA	2.15	0.47
1:B:239:GLY:N	1:B:256:ASN:ND2	2.63	0.46
1:B:290:LEU:HD11	1:B:323:ILE:HG13	1.97	0.46
1:B:311:TRP:HE1	1:B:390:LYS:CE	2.28	0.46
1:D:342:ILE:N	1:D:343:PRO:HD2	2.30	0.46
1:A:65:SER:C	1:A:67:PHE:H	2.19	0.46
1:A:97:ARG:NH2	1:B:344:ASP:CG	2.59	0.46
1:B:343:PRO:O	1:B:347:LEU:N	2.39	0.46
1:B:308:LYS:HG3	1:B:369:ALA:HB1	1.97	0.46
1:C:41:ASN:O	1:C:44:LYS:HG2	2.16	0.46
1:D:226:LEU:O	1:D:227:ASP:CB	2.64	0.46
1:B:138:CYS:C	1:B:140:LEU:H	2.18	0.46
1:B:242:VAL:O	1:B:243:SER:C	2.55	0.46
1:A:187:ALA:HB3	1:A:192:TYR:HB2	1.98	0.46
1:C:294:VAL:O	1:C:298:TRP:HD1	1.99	0.46
1:A:59:ASN:O	1:A:63:LEU:HG	2.17	0.45
1:B:53:ARG:NH1	1:B:158:SER:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HD12	1:B:348:MET:HE3	1.98	0.45
1:C:137:SER:O	1:C:140:LEU:HB2	2.17	0.45
1:A:248:LYS:C	1:A:249:TYR:CD1	2.89	0.45
1:B:320:VAL:HG13	1:B:388:PHE:HB2	1.99	0.45
1:B:48:ILE:N	1:B:49:PRO:HD2	2.32	0.45
1:C:303:CYS:HB3	1:C:365:LEU:HD13	1.98	0.45
1:A:50:MET:HB3	1:B:166:PHE:HB3	1.99	0.45
1:B:232:LEU:O	1:B:289:MET:HA	2.17	0.45
1:B:234:VAL:HB	1:B:291:LEU:CD2	2.47	0.45
1:B:238:ILE:O	1:B:269:TYR:HE2	1.99	0.45
1:B:366:GLY:O	1:B:371:PHE:HB2	2.17	0.45
1:C:214:VAL:HG13	1:C:383:LEU:HD21	1.98	0.44
1:A:234:VAL:HB	1:A:291:LEU:HD23	1.99	0.44
1:A:265:VAL:O	1:A:266:ALA:C	2.55	0.44
1:C:285:LYS:HA	1:C:313:SER:O	2.16	0.44
1:C:225:PHE:C	1:C:226:LEU:O	2.52	0.44
1:B:347:LEU:O	1:B:351:ASN:C	2.55	0.44
1:A:52:LEU:O	1:A:55:ALA:HB3	2.18	0.44
1:A:373:LYS:HB3	1:A:389:HIS:HB2	1.99	0.44
1:C:232:LEU:CD2	1:C:283:VAL:HG13	2.48	0.44
1:C:72:LYS:HA	1:C:131:TYR:O	2.17	0.44
1:C:179:VAL:O	1:C:182:GLU:N	2.51	0.44
1:B:107:ILE:O	1:B:134:THR:CG2	2.66	0.44
1:A:256:ASN:HD22	1:A:274:HIS:CE1	2.35	0.43
1:C:97:ARG:NE	1:D:348:MET:HE1	2.33	0.43
1:D:90:GLU:O	1:D:92:ALA:N	2.51	0.43
1:A:97:ARG:NH2	1:B:344:ASP:OD1	2.52	0.43
1:A:358:THR:N	1:A:361:GLU:OE2	2.48	0.43
1:B:41:ASN:O	1:B:44:LYS:HG2	2.18	0.43
1:C:59:ASN:OD1	1:C:62:GLN:HB2	2.16	0.43
1:C:210:PHE:HE1	1:D:39:THR:HG21	1.83	0.43
1:B:162:VAL:O	1:B:165:SER:HB2	2.19	0.43
1:C:152:GLU:OE1	1:C:152:GLU:N	2.46	0.43
1:A:90:GLU:O	1:A:91:ALA:C	2.56	0.43
1:A:132:GLY:O	1:A:133:LEU:O	2.37	0.43
1:A:281:GLU:O	1:A:309:ASN:ND2	2.51	0.43
1:B:295:LEU:HD11	1:B:322:ILE:CD1	2.48	0.43
1:D:254:GLY:O	1:D:272:VAL:HA	2.19	0.43
1:D:347:LEU:O	1:D:351:ASN:N	2.46	0.43
1:A:267:PRO:HG2	1:A:269:TYR:CZ	2.54	0.43
1:B:351:ASN:O	1:B:353:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:NH1	1:C:158:SER:OG	2.51	0.43
1:A:181:PHE:CE1	1:A:189:ILE:HA	2.54	0.43
1:C:296:HIS:HD2	1:C:297:ASP:N	2.17	0.43
1:B:214:VAL:HG21	1:B:293:TRP:CZ2	2.54	0.43
1:B:308:LYS:HE2	1:B:369:ALA:HA	2.01	0.43
1:C:97:ARG:HE	1:D:348:MET:HE1	1.83	0.43
1:C:232:LEU:HD21	1:C:283:VAL:HG13	2.00	0.43
1:D:286:GLY:O	1:D:315:PRO:HD2	2.19	0.42
1:C:248:LYS:HG2	1:C:249:TYR:CE2	2.54	0.42
1:B:223:ASP:O	1:B:225:PHE:N	2.52	0.42
1:C:326:VAL:HB	1:C:384:HIS:ND1	2.34	0.42
1:A:260:PRO:O	1:A:264:SER:N	2.49	0.42
1:D:94:TYR:O	1:D:97:ARG:N	2.52	0.42
1:B:267:PRO:CG	1:B:269:TYR:OH	2.66	0.42
1:B:287:GLN:HA	1:B:315:PRO:HD2	2.01	0.42
1:D:63:LEU:N	1:D:63:LEU:HD23	2.35	0.42
1:D:157:THR:HG22	1:D:346:LEU:HD11	2.01	0.42
1:A:358:THR:HG22	1:A:361:GLU:CD	2.32	0.42
1:A:145:GLU:O	1:C:248:LYS:HE3	2.20	0.42
1:D:74:SER:OG	1:D:77:GLU:HG3	2.19	0.42
1:A:135:ASN:O	1:A:138:CYS:HB2	2.20	0.42
1:C:61:PHE:CE1	1:C:108:LEU:HD21	2.55	0.42
1:B:371:PHE:CD2	1:B:388:PHE:HB3	2.55	0.41
1:A:199:MET:CE	1:A:203:PHE:CE2	3.03	0.41
1:B:374:THR:O	1:B:376:PRO:HD3	2.20	0.41
1:D:74:SER:HA	1:D:130:LEU:HD23	2.00	0.41
1:D:343:PRO:O	1:D:347:LEU:N	2.44	0.41
1:B:168:LYS:HD2	1:B:183:VAL:CG1	2.51	0.41
1:D:65:SER:CB	1:D:141:VAL:HG11	2.51	0.41
1:A:375:ILE:HA	1:A:376:PRO:HD2	1.83	0.41
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.90	0.41
1:B:286:GLY:O	1:B:315:PRO:HD2	2.19	0.41
1:D:362:TYR:O	1:D:363:ASP:C	2.58	0.41
1:D:363:ASP:O	1:D:364:ASP:C	2.57	0.41
1:C:59:ASN:CG	1:C:62:GLN:HB3	2.41	0.41
1:A:35:TYR:O	1:A:38:GLU:N	2.54	0.41
1:D:62:GLN:HA	1:D:141:VAL:HG13	2.02	0.41
1:B:240:THR:HG23	1:B:269:TYR:OH	2.21	0.41
1:C:212:ILE:O	1:C:216:GLU:HG3	2.21	0.41
1:D:58:LEU:C	1:D:60:VAL:N	2.74	0.41
1:A:176:LYS:HA	1:B:88:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ALA:O	1:C:92:ALA:C	2.59	0.40
1:A:341:LEU:HD21	1:B:100:ARG:HD2	2.02	0.40
1:B:262:VAL:O	1:B:265:VAL:HG22	2.21	0.40
1:B:380:SER:OG	1:B:381:ASN:OD1	2.39	0.40
1:B:232:LEU:N	1:B:288:ASN:O	2.43	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	338/393 (86%)	272 (80%)	55 (16%)	11 (3%)	4	17
1	B	338/393 (86%)	260 (77%)	63 (19%)	15 (4%)	2	12
1	C	338/393 (86%)	295 (87%)	37 (11%)	6 (2%)	8	30
1	D	342/393 (87%)	284 (83%)	46 (14%)	12 (4%)	3	17
All	All	1356/1572 (86%)	1111 (82%)	201 (15%)	44 (3%)	4	18

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	B	60	VAL
1	B	70	ASP
1	D	59	ASN
1	D	91	ALA
1	D	281	GLU
1	D	301	GLU
1	A	35	TYR
1	A	91	ALA
1	A	174	GLU

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Mol	Chain	Res	Type
1	B	59	ASN
1	B	139	CYS
1	B	224	GLY
1	B	309	ASN
1	C	372	ILE
1	D	145	GLU
1	A	66	LYS
1	A	133	LEU
1	A	139	CYS
1	A	167	PHE
1	A	208	ALA
1	B	227	ASP
1	B	383	LEU
1	C	83	PRO
1	C	301	GLU
1	C	381	ASN
1	D	135	ASN
1	B	333	ASN
1	C	190	PHE
1	D	227	ASP
1	D	360	SER
1	A	59	ASN
1	B	86	LYS
1	B	135	ASN
1	C	378	PRO
1	A	226	LEU
1	B	145	GLU
1	D	60	VAL
1	B	386	ILE
1	B	352	PRO
1	D	234	VAL
1	D	284	PRO
1	B	103	GLY
1	D	366	GLY

### 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	258/333 (78%)	235 (91%)	23 (9%)	9	31
1	B	238/333 (72%)	215 (90%)	23 (10%)	8	27
1	C	245/333 (74%)	228 (93%)	17 (7%)	15	42
1	D	246/333 (74%)	223 (91%)	23 (9%)	9	29
All	All	987/1332 (74%)	901 (91%)	86 (9%)	10	33

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	CYS
1	A	36	LEU
1	A	48	ILE
1	A	53	ARG
1	A	65	SER
1	A	66	LYS
1	A	76	SER
1	A	110	VAL
1	A	131	TYR
1	A	149	SER
1	A	158	SER
1	A	189	ILE
1	A	195	THR
1	A	207	MET
1	A	209	VAL
1	A	241	SER
1	A	243	SER
1	A	279	MET
1	A	289	MET
1	A	296	HIS
1	A	334	ASN
1	A	336	GLU
1	A	358	THR
1	B	37	SER
1	B	38	GLU
1	B	53	ARG
1	B	74	SER
1	B	76	SER
1	B	84	ASN
1	B	98	ILE
1	B	110	VAL
1	B	112	THR
1	B	134	THR

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Mol	Chain	Res	Type
1	B	136	SER
1	B	146	ASP
1	B	161	VAL
1	B	167	PHE
1	B	176	LYS
1	B	178	SER
1	B	195	THR
1	B	201	GLN
1	B	218	VAL
1	B	241	SER
1	B	287	GLN
1	B	296	HIS
1	B	344	ASP
1	C	34	CYS
1	C	38	GLU
1	C	44	LYS
1	C	56	MET
1	C	84	ASN
1	C	106	SER
1	C	205	ASP
1	C	211	SER
1	C	241	SER
1	C	243	SER
1	C	268	GLN
1	C	296	HIS
1	C	302	ARG
1	C	304	VAL
1	C	347	LEU
1	C	348	MET
1	C	355	LYS
1	D	34	CYS
1	D	53	ARG
1	D	56	MET
1	D	66	LYS
1	D	72	LYS
1	D	84	ASN
1	D	110	VAL
1	D	112	THR
1	D	127	HIS
1	D	146	ASP
1	D	153	GLU
1	D	156	PHE

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Mol	Chain	Res	Type
1	D	189	ILE
1	D	200	ASN
1	D	209	VAL
1	D	210	PHE
1	D	226	LEU
1	D	240	THR
1	D	283	VAL
1	D	289	MET
1	D	296	HIS
1	D	305	LYS
1	D	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	342/393 (87%)	-0.30	0 100 100	36, 60, 95, 124	52 (15%)
1	B	342/393 (87%)	-0.37	0 100 100	42, 72, 102, 121	95 (27%)
1	C	342/393 (87%)	-0.35	1 (0%) 94 85	38, 63, 92, 121	124 (36%)
1	D	346/393 (88%)	-0.41	0 100 100	36, 63, 89, 118	139 (40%)
All	All	1372/1572 (87%)	-0.36	1 (0%) 95 91	36, 65, 97, 124	410 (29%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	ALA	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.