



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:15 AM UTC

PDB ID : 1E5X / pdb_00001e5x
Title : Structure of threonine synthase from Arabidopsis thaliana
Authors : Thomazeau, K.; Curien, G.; Dumas, R.; Biou, V.
Deposited on : 2000-08-04
Resolution : 2.25 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

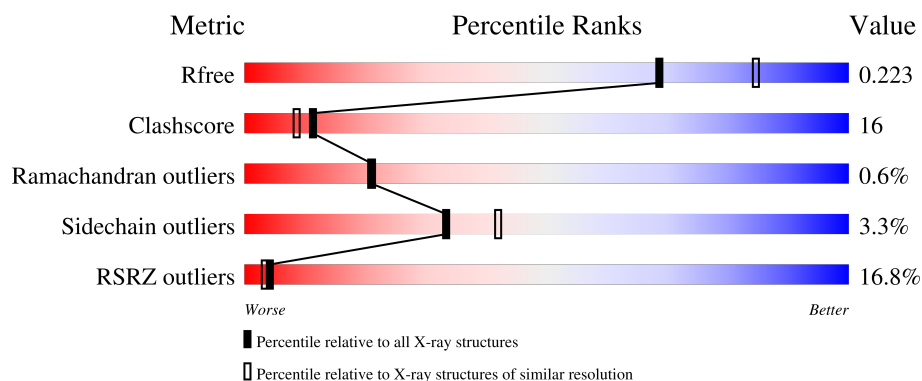
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	486	16% 67% 23% • 7%
1	B	486	13% 66% 20% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7289 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 THREONINE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	Se	0	2	0
			3514	2236	592	664	9	13			
1	B	433	Total	C	N	O	S	Se	0	3	0
			3387	2158	569	638	9	13			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	MSO	MET	modified residue	UNP Q39144
B	309	MSO	MET	modified residue	UNP Q39144
A	77	MSE	MET	modified residue	UNP Q39144
A	146	MSE	MET	modified residue	UNP Q39144
A	167	MSE	MET	modified residue	UNP Q39144
A	180	MSE	MET	modified residue	UNP Q39144
A	221	MSE	MET	modified residue	UNP Q39144
A	245	MSE	MET	modified residue	UNP Q39144
A	322	MSE	MET	modified residue	UNP Q39144
A	388	MSE	MET	modified residue	UNP Q39144
A	391	MSE	MET	modified residue	UNP Q39144
A	399	MSE	MET	modified residue	UNP Q39144
A	453	MSE	MET	modified residue	UNP Q39144
A	472	MSE	MET	modified residue	UNP Q39144
B	77	MSE	MET	modified residue	UNP Q39144
B	146	MSE	MET	modified residue	UNP Q39144
B	167	MSE	MET	modified residue	UNP Q39144
B	180	MSE	MET	modified residue	UNP Q39144
B	221	MSE	MET	modified residue	UNP Q39144
B	245	MSE	MET	modified residue	UNP Q39144
B	322	MSE	MET	modified residue	UNP Q39144
B	388	MSE	MET	modified residue	UNP Q39144
B	391	MSE	MET	modified residue	UNP Q39144
B	399	MSE	MET	modified residue	UNP Q39144
B	453	MSE	MET	modified residue	UNP Q39144

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	472	MSE	MET	modified residue	UNP Q39144

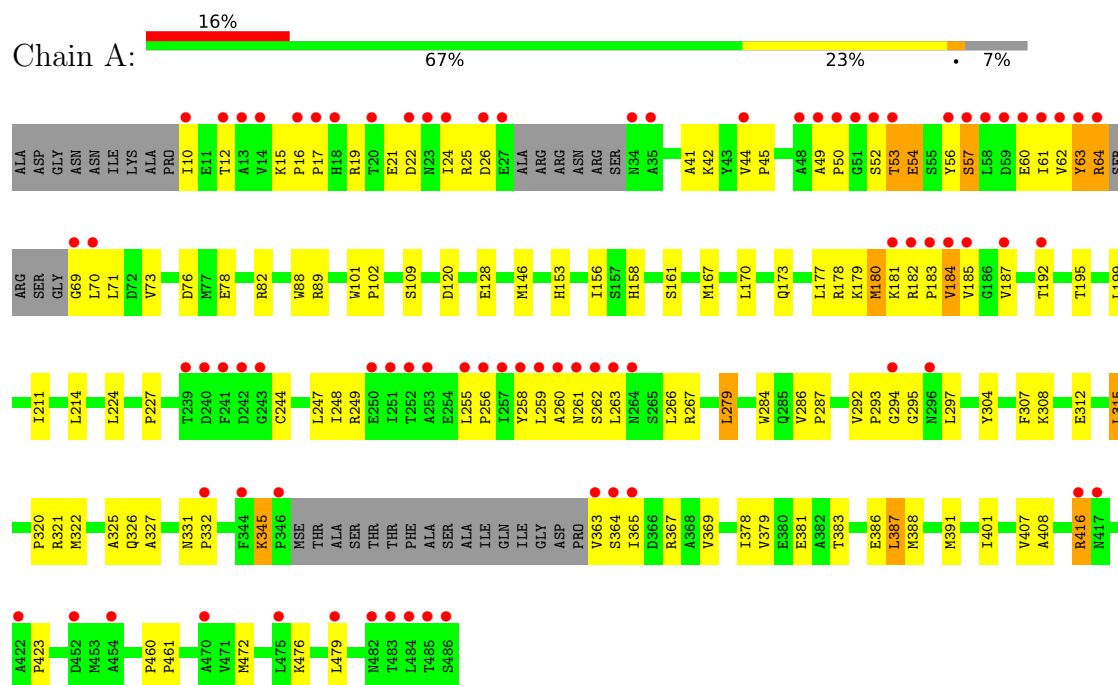
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	203	Total 203	O 203	0	0
2	B	185	Total 185	O 185	0	0

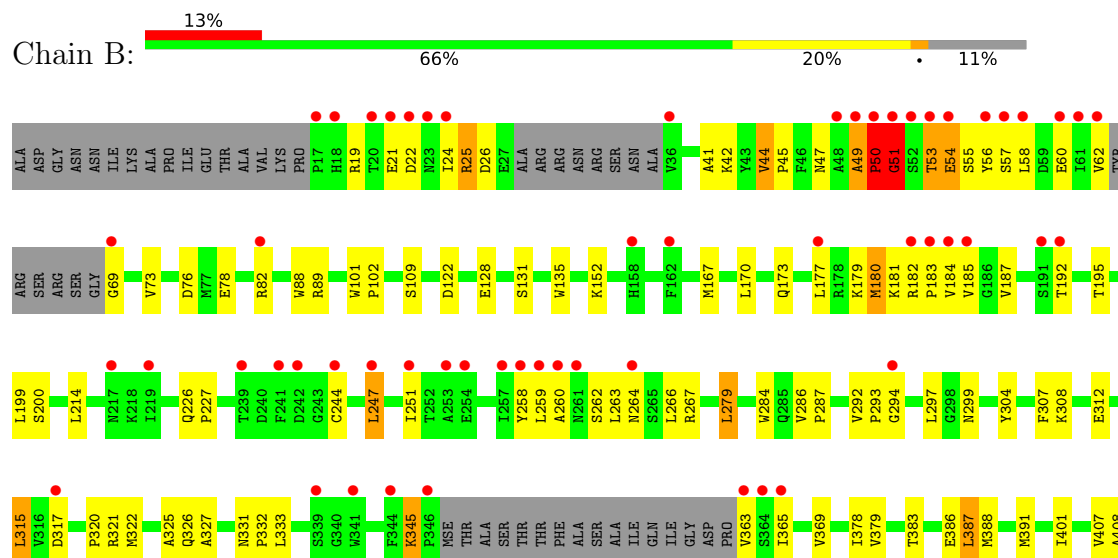
3 Residue-property plots

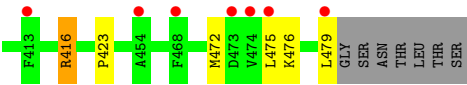
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: THREONINE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.76Å 62.14Å 76.59Å 109.48° 97.61° 112.74°	Depositor
Resolution (Å)	29.81 – 2.25 29.81 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.81-2.25) 98.7 (29.81-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.38 (at 2.24Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.243 0.227 , 0.223	Depositor DCC
R_{free} test set	4136 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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

5.1 Standard geometry

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

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	0.43	0/3571	0.92	10/4822 (0.2%)
1	B	0.41	0/3442	0.90	8/4646 (0.2%)
All	All	0.42	0/7013	0.91	18/9468 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	SER	N-CA-C	6.34	118.50	110.33
1	A	286	VAL	N-CA-C	6.18	113.94	108.63
1	B	292	VAL	N-CA-C	5.99	114.01	107.60
1	B	286	VAL	N-CA-C	5.97	113.76	108.63
1	B	25	ARG	N-CA-C	-5.85	105.24	112.38
1	A	321	ARG	N-CA-C	-5.80	101.90	110.48
1	A	180	MSE	N-CA-C	-5.73	106.62	113.21
1	A	158	HIS	N-CA-C	5.71	117.50	111.28
1	A	109	SER	N-CA-C	-5.64	106.24	113.01
1	A	292	VAL	N-CA-C	5.62	113.62	107.60
1	B	180	MSE	N-CA-C	-5.53	106.85	113.21
1	A	63	TYR	N-CA-C	5.50	116.43	108.34
1	B	51	GLY	N-CA-C	5.50	126.22	113.18
1	B	321	ARG	N-CA-C	-5.41	102.47	110.48
1	B	327	ALA	N-CA-C	-5.28	102.67	110.48
1	B	109	SER	N-CA-C	-5.19	106.78	113.01
1	A	327	ALA	N-CA-C	-5.04	103.02	110.48
1	A	57	SER	N-CA-C	-5.04	107.08	113.18

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	3514	0	3445	129	0
1	B	3387	0	3314	100	0
2	A	203	0	0	7	0
2	B	185	0	0	4	0
All	All	7289	0	6759	222	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 16.

All (222) 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:A:56:TYR:OH	1:A:73:VAL:HG13	1.49	1.12
1:B:56:TYR:OH	1:B:73:VAL:HG13	1.53	1.09
1:A:62:VAL:HG12	1:A:64:ARG:HH12	1.41	0.85
1:B:294:GLY:HA3	1:B:326:GLN:HE22	1.44	0.81
1:A:391:MSE:HA	1:A:401:ILE:HD11	1.65	0.79
1:A:178:ARG:HD3	2:A:2102:HOH:O	1.83	0.78
1:B:24:ILE:HD13	1:B:101:TRP:O	1.84	0.78
1:B:391:MSE:HA	1:B:401:ILE:HD11	1.66	0.77
1:B:173:GLN:HG2	1:B:266:LEU:HD21	1.67	0.77
1:B:22:ASP:HA	1:B:25:ARG:HH12	1.49	0.77
1:A:57:SER:HA	1:A:177:LEU:HD21	1.67	0.75
1:A:294:GLY:HA3	1:A:326:GLN:HE22	1.50	0.74
1:B:22:ASP:HA	1:B:25:ARG:NH1	2.01	0.74
1:A:185:VAL:HG12	1:B:479:LEU:HD22	1.70	0.73
1:A:54:GLU:HG3	1:A:60:GLU:HG3	1.69	0.73
1:B:304:TYR:HB2	1:B:322:MSE:HE1	1.70	0.73
1:B:54:GLU:HB3	1:B:60:GLU:HG3	1.72	0.72
1:A:63:TYR:CD1	1:A:64:ARG:HG3	2.25	0.71
1:A:173:GLN:HG2	1:A:266:LEU:HD21	1.72	0.71
1:A:41:ALA:HB3	1:A:56:TYR:HE2	1.53	0.71
1:B:294:GLY:HA3	1:B:326:GLN:NE2	2.05	0.71
1:B:54:GLU:CB	1:B:60:GLU:HG3	2.22	0.69
1:A:19:ARG:HG2	1:A:22:ASP:OD2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HD13	1:A:101:TRP:O	1.93	0.68
1:B:264:ASN:O	1:B:267:ARG:HG2	1.93	0.68
1:B:294:GLY:CA	1:B:326:GLN:HE22	2.06	0.68
1:B:21:GLU:OE2	2:B:2003:HOH:O	2.12	0.68
1:A:345:LYS:HA	1:A:345:LYS:HE3	1.76	0.67
1:A:24:ILE:HD11	1:A:101:TRP:HD1	1.59	0.67
1:A:331:ASN:HB2	1:A:332:PRO:HD2	1.74	0.67
1:A:19:ARG:HD2	2:A:2009:HOH:O	1.94	0.67
1:A:294:GLY:CA	1:A:326:GLN:HE22	2.08	0.67
1:A:128:GLU:CD	1:A:128:GLU:H	2.03	0.66
1:A:15:LYS:HB3	1:A:17:PRO:HD2	1.77	0.66
1:A:64:ARG:HD2	1:A:64:ARG:O	1.94	0.66
1:B:345:LYS:HE3	1:B:345:LYS:HA	1.76	0.66
1:B:331:ASN:HB2	1:B:332:PRO:HD2	1.75	0.66
1:B:128:GLU:CD	1:B:128:GLU:H	2.03	0.66
1:A:63:TYR:HD1	1:A:64:ARG:H	1.40	0.66
1:A:62:VAL:HG13	1:A:69:GLY:O	1.96	0.66
1:A:294:GLY:HA3	1:A:326:GLN:NE2	2.11	0.65
1:A:54:GLU:CG	1:A:60:GLU:HG3	2.27	0.65
1:A:304:TYR:HB2	1:A:322:MSE:HE1	1.78	0.65
1:B:179:LYS:C	1:B:181:LYS:H	2.05	0.64
1:B:78:GLU:HG2	1:B:82:ARG:HH12	1.62	0.64
1:A:179:LYS:C	1:A:181:LYS:H	2.04	0.64
1:A:78:GLU:HG2	1:A:82:ARG:HH12	1.62	0.64
1:B:267:ARG:HG3	1:B:267:ARG:HH11	1.63	0.63
1:B:416:ARG:NH2	1:B:423:PRO:HD3	2.14	0.63
1:B:41:ALA:HB3	1:B:56:TYR:HE2	1.63	0.63
1:A:187:VAL:HG11	1:A:199:LEU:HD11	1.80	0.62
1:A:56:TYR:HH	1:A:73:VAL:HG13	1.63	0.62
1:B:170:LEU:C	1:B:170:LEU:HD23	2.25	0.62
1:A:64:ARG:HD2	1:A:64:ARG:C	2.25	0.62
1:A:63:TYR:HD1	1:A:64:ARG:HG3	1.65	0.60
1:A:161:SER:HB3	2:A:2097:HOH:O	2.01	0.60
1:A:170:LEU:C	1:A:170:LEU:HD23	2.26	0.60
1:B:387:LEU:HD22	1:B:388:MSE:HG2	1.83	0.60
1:B:187:VAL:HG11	1:B:199:LEU:HD11	1.84	0.59
1:B:49:ALA:HB1	1:B:50:PRO:CD	2.33	0.59
1:B:181:LYS:O	1:B:183:PRO:HD3	2.01	0.59
1:A:54:GLU:CB	1:A:60:GLU:HG3	2.33	0.59
1:A:63:TYR:HD1	1:A:64:ARG:N	2.01	0.59
1:A:24:ILE:HG21	1:A:101:TRP:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:O	1:A:369:VAL:HG23	2.02	0.58
1:A:259:LEU:O	1:A:262:SER:HB3	2.04	0.58
1:A:16:PRO:N	1:A:17:PRO:HD2	2.19	0.58
1:A:293:PRO:HG3	1:A:408:ALA:HB2	1.84	0.58
1:B:287:PRO:O	1:B:320:PRO:HB3	2.04	0.58
1:A:62:VAL:HG12	1:A:63:TYR:H	1.69	0.58
1:A:416:ARG:NH2	1:A:423:PRO:HD3	2.19	0.58
1:A:287:PRO:O	1:A:320:PRO:HB3	2.04	0.57
1:A:479:LEU:HD22	1:B:185:VAL:HG12	1.86	0.57
1:B:365:ILE:O	1:B:369:VAL:HG23	2.04	0.57
1:A:64:ARG:NH2	1:A:69:GLY:HA3	2.19	0.57
1:A:62:VAL:CG1	1:A:64:ARG:HH22	2.18	0.56
1:A:76:ASP:OD1	1:A:78:GLU:HB3	2.05	0.56
1:A:24:ILE:HD12	1:A:120:ASP:OD2	2.04	0.56
1:A:199:LEU:HD22	1:A:260:ALA:HB2	1.88	0.56
1:B:76:ASP:OD1	1:B:78:GLU:HB3	2.06	0.56
1:B:24:ILE:HG23	2:B:2044:HOH:O	2.04	0.56
1:B:58:LEU:HD23	1:B:60:GLU:OE2	2.06	0.56
1:B:41:ALA:HB1	1:B:56:TYR:OH	2.06	0.55
1:A:16:PRO:HG2	1:A:17:PRO:HD3	1.88	0.55
1:B:49:ALA:HB1	1:B:50:PRO:HD2	1.88	0.55
1:A:185:VAL:HG11	1:B:479:LEU:HD13	1.87	0.55
1:A:181:LYS:O	1:A:183:PRO:HD3	2.07	0.55
1:B:24:ILE:HD11	1:B:101:TRP:HD1	1.71	0.55
1:A:60:GLU:O	1:A:61:ILE:HD13	2.07	0.55
1:B:62:VAL:HG13	1:B:69:GLY:O	2.07	0.55
1:B:199:LEU:HD22	1:B:260:ALA:HB2	1.89	0.54
1:A:297:LEU:CD1	1:A:365:ILE:HG22	2.38	0.54
1:B:42:LYS:HD2	1:B:53:THR:OG1	2.07	0.54
1:A:88:TRP:CB	1:A:315:LEU:HD11	2.37	0.54
1:B:57:SER:HA	1:B:177:LEU:HD21	1.90	0.54
1:A:41:ALA:HB3	1:A:56:TYR:CE2	2.39	0.54
1:A:308:LYS:HE3	1:A:312:GLU:OE2	2.08	0.54
1:B:88:TRP:CB	1:B:315:LEU:HD11	2.38	0.54
1:A:24:ILE:CD1	1:A:101:TRP:HD1	2.20	0.54
1:A:78:GLU:HG2	1:A:82:ARG:NH1	2.23	0.53
1:A:192:THR:HG22	1:A:214:LEU:HD11	1.89	0.53
1:B:78:GLU:HG2	1:B:82:ARG:NH1	2.24	0.53
1:A:49:ALA:HB1	1:A:50:PRO:HD2	1.91	0.53
1:A:62:VAL:HG11	1:A:64:ARG:HH22	1.73	0.53
1:B:259:LEU:O	1:B:262:SER:HB3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:HH	1:A:69:GLY:N	2.08	0.52
1:B:263:LEU:N	1:B:263:LEU:HD12	2.25	0.52
1:B:279:LEU:HD13	1:B:307:PHE:HE1	1.74	0.52
1:A:387:LEU:HD22	1:A:388:MSE:HG2	1.91	0.51
1:B:41:ALA:HB3	1:B:56:TYR:CE2	2.45	0.51
1:B:308:LYS:HE3	1:B:312:GLU:OE2	2.11	0.51
1:B:325:ALA:HB1	1:B:407:VAL:HG12	1.93	0.51
1:A:279:LEU:HD13	1:A:307:PHE:HE1	1.75	0.51
1:B:55:SER:HB3	1:B:58:LEU:HD13	1.93	0.51
1:A:49:ALA:HB1	1:A:50:PRO:CD	2.42	0.51
1:A:167:MSE:CE	1:A:195:THR:HG23	2.41	0.50
1:A:383:THR:OG1	1:A:386:GLU:HG3	2.12	0.50
1:A:41:ALA:HB1	1:A:56:TYR:OH	2.10	0.50
1:A:24:ILE:HG23	2:A:2007:HOH:O	2.11	0.50
1:B:24:ILE:HG21	1:B:101:TRP:O	2.12	0.50
1:A:21:GLU:OE2	2:A:2008:HOH:O	2.20	0.49
1:A:479:LEU:HD13	1:B:185:VAL:HG11	1.94	0.49
1:A:16:PRO:N	1:A:17:PRO:CD	2.75	0.49
1:A:62:VAL:HG12	1:A:63:TYR:N	2.27	0.49
1:A:63:TYR:CD1	1:A:64:ARG:N	2.77	0.49
1:A:472:MSE:CE	1:A:476:LYS:HE2	2.43	0.49
1:A:258:TYR:HB3	1:A:263:LEU:HD11	1.94	0.49
1:B:267:ARG:HG3	1:B:267:ARG:NH1	2.28	0.49
1:A:63:TYR:HE2	1:A:70:LEU:O	1.96	0.48
1:B:304:TYR:HB2	1:B:322:MSE:CE	2.41	0.48
1:B:416:ARG:HH22	1:B:423:PRO:HD3	1.78	0.48
1:A:182:ARG:O	1:A:184:VAL:HG23	2.13	0.48
1:A:416:ARG:HH22	1:A:423:PRO:HD3	1.79	0.48
1:A:167:MSE:SE	1:A:267:ARG:HD3	2.63	0.48
1:A:263:LEU:HD12	1:A:263:LEU:N	2.29	0.48
1:A:63:TYR:CE2	1:A:70:LEU:O	2.67	0.48
1:B:182:ARG:O	1:B:184:VAL:HG23	2.14	0.48
1:A:179:LYS:C	1:A:181:LYS:N	2.72	0.47
1:A:45:PRO:HA	1:A:63:TYR:CD2	2.49	0.47
1:A:88:TRP:HB3	1:A:315:LEU:HD11	1.96	0.47
1:B:258:TYR:HB3	1:B:263:LEU:HD11	1.96	0.47
1:A:387:LEU:C	1:A:387:LEU:HD23	2.40	0.47
1:B:363:VAL:HG12	1:B:363:VAL:O	2.15	0.47
1:A:249:ARG:HG2	1:A:249:ARG:HH11	1.80	0.46
1:A:24:ILE:CG2	2:A:2007:HOH:O	2.63	0.46
1:B:294:GLY:CA	1:B:326:GLN:NE2	2.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:PRO:HG3	1:B:408:ALA:HB2	1.97	0.46
1:B:19:ARG:HG2	1:B:22:ASP:OD2	2.16	0.46
1:A:192:THR:HG22	1:A:214:LEU:CD1	2.45	0.46
1:B:192:THR:HG22	1:B:214:LEU:HD11	1.96	0.46
1:A:22:ASP:OD1	1:A:25:ARG:NH2	2.49	0.46
1:A:42:LYS:HD2	1:A:53:THR:HG21	1.98	0.46
1:A:71:LEU:O	1:A:367:ARG:NH2	2.49	0.46
1:A:211:ILE:HD13	1:B:475:LEU:HD22	1.97	0.45
1:B:88:TRP:HB2	1:B:315:LEU:HD11	1.97	0.45
1:A:19:ARG:HB2	1:B:135:TRP:CZ2	2.51	0.45
1:B:49:ALA:O	1:B:51:GLY:N	2.49	0.45
1:A:146:MSE:SE	1:A:416:ARG:HD2	2.65	0.45
1:A:326:GLN:O	1:A:381:GLU:HA	2.16	0.45
1:A:363:VAL:O	1:A:364:SER:HB3	2.16	0.45
1:B:122:ASP:OD1	1:B:179:LYS:HD2	2.17	0.45
1:A:315:LEU:N	1:A:315:LEU:CD2	2.80	0.45
1:B:279:LEU:HD13	1:B:307:PHE:CE1	2.52	0.45
1:B:49:ALA:C	1:B:51:GLY:H	2.24	0.44
1:A:15:LYS:C	1:A:17:PRO:HD2	2.42	0.44
1:B:50:PRO:O	1:B:51:GLY:O	2.36	0.44
1:B:89:ARG:HD2	1:B:284:TRP:CD1	2.52	0.44
1:A:56:TYR:CE1	1:A:73:VAL:HG22	2.52	0.44
1:B:294:GLY:C	1:B:326:GLN:HE22	2.26	0.44
1:B:297:LEU:CD1	1:B:365:ILE:HG22	2.47	0.44
1:A:63:TYR:O	1:A:64:ARG:C	2.60	0.44
1:B:299:ASN:ND2	2:B:2120:HOH:O	2.51	0.44
1:A:153:HIS:HB3	1:A:156:ILE:HG13	1.99	0.43
1:B:44:VAL:HG13	1:B:45:PRO:HD2	2.00	0.43
1:A:294:GLY:C	1:A:326:GLN:HE22	2.25	0.43
1:A:325:ALA:HB1	1:A:407:VAL:HG12	1.99	0.43
1:B:200:SER:HB2	2:B:2101:HOH:O	2.18	0.43
1:A:64:ARG:O	1:A:64:ARG:NH1	2.52	0.43
1:B:333:LEU:HD13	1:B:365:ILE:HB	2.00	0.43
1:A:10:ILE:HG12	1:A:10:ILE:O	2.19	0.43
1:A:24:ILE:C	1:A:26:ASP:N	2.71	0.43
1:A:62:VAL:HG13	1:A:69:GLY:C	2.43	0.43
1:B:179:LYS:C	1:B:181:LYS:N	2.73	0.43
1:A:42:LYS:HD2	1:A:53:THR:CG2	2.49	0.43
1:A:294:GLY:CA	1:A:326:GLN:NE2	2.77	0.43
1:B:472:MSE:O	1:B:476:LYS:HG2	2.19	0.43
1:A:279:LEU:HD13	1:A:307:PHE:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLY:O	1:A:295:GLY:C	2.61	0.42
1:B:315:LEU:CD2	1:B:315:LEU:N	2.82	0.42
1:B:378:ILE:HG22	1:B:379:VAL:N	2.34	0.42
1:A:89:ARG:HG3	1:A:315:LEU:HD13	2.00	0.42
1:A:261:ASN:OD1	1:A:267:ARG:NH2	2.52	0.42
1:B:89:ARG:HG3	1:B:315:LEU:HD13	2.01	0.42
1:A:88:TRP:HB2	1:A:315:LEU:HD11	2.00	0.42
1:A:224:LEU:O	1:A:227:PRO:HD2	2.20	0.42
1:B:383:THR:OG1	1:B:386:GLU:HG3	2.20	0.42
1:A:244:CYS:O	1:A:248:ILE:HG13	2.20	0.42
1:A:89:ARG:HD2	1:A:284:TRP:CD1	2.55	0.42
1:B:56:TYR:CE1	1:B:73:VAL:HG22	2.55	0.42
1:A:472:MSE:O	1:A:476:LYS:HG2	2.20	0.42
1:B:88:TRP:HB3	1:B:315:LEU:HD11	2.02	0.42
1:B:128:GLU:CD	1:B:128:GLU:N	2.76	0.42
1:B:387:LEU:C	1:B:387:LEU:HD23	2.45	0.42
1:A:180:MSE:HB2	1:A:182:ARG:HG2	2.02	0.41
1:A:460:PRO:HA	1:A:461:PRO:HD3	1.96	0.41
1:B:167:MSE:CE	1:B:195:THR:HG23	2.49	0.41
1:A:267:ARG:HD2	2:A:2140:HOH:O	2.20	0.41
1:B:263:LEU:HD12	1:B:263:LEU:H	1.84	0.41
1:B:192:THR:HG22	1:B:214:LEU:CD1	2.51	0.41
1:B:226:GLN:HB2	1:B:227:PRO:HD3	2.01	0.41
1:A:24:ILE:C	1:A:26:ASP:H	2.29	0.41
1:A:128:GLU:CD	1:A:128:GLU:N	2.77	0.41
1:A:185:VAL:CG1	1:B:479:LEU:HD13	2.50	0.41
1:B:180:MSE:HB2	1:B:182:ARG:HG2	2.02	0.41
1:A:378:ILE:HG22	1:A:379:VAL:N	2.36	0.41
1:B:56:TYR:HH	1:B:73:VAL:HG13	1.76	0.41
1:B:131:SER:OG	1:B:152:LYS:HE3	2.21	0.41
1:B:317[A]:ASP:O	1:B:317[A]:ASP:CG	2.64	0.41
1:B:247:LEU:O	1:B:251:ILE:HG12	2.20	0.40
1:B:54:GLU:CG	1:B:60:GLU:HG3	2.51	0.40
1:A:255:LEU:HA	1:A:256:PRO:HD3	1.89	0.40
1:B:24:ILE:C	1:B:26:ASP:N	2.77	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	444/486 (91%)	410 (92%)	33 (7%)	1 (0%)	43	50
1	B	427/486 (88%)	396 (93%)	27 (6%)	4 (1%)	14	12
All	All	871/972 (90%)	806 (92%)	60 (7%)	5 (1%)	21	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	GLY
1	B	49	ALA
1	B	50	PRO
1	B	47	ASN
1	A	184	VAL

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	378/389 (97%)	366 (97%)	12 (3%)	34	43
1	B	364/389 (94%)	352 (97%)	12 (3%)	33	42
All	All	742/778 (95%)	718 (97%)	24 (3%)	33	43

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	44	VAL
1	A	53	THR
1	A	54	GLU
1	A	64	ARG
1	A	102	PRO
1	A	247	LEU
1	A	279	LEU
1	A	315	LEU
1	A	345	LYS
1	A	387	LEU
1	A	416	ARG
1	B	44	VAL
1	B	50	PRO
1	B	53	THR
1	B	54	GLU
1	B	102	PRO
1	B	244	CYS
1	B	247	LEU
1	B	279	LEU
1	B	315	LEU
1	B	345	LYS
1	B	387	LEU
1	B	416	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	230	ASN
1	A	299	ASN
1	A	326	GLN
1	A	376	ASN
1	B	153	HIS
1	B	230	ASN
1	B	271	GLN
1	B	299	ASN
1	B	326	GLN
1	B	376	ASN

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	MSO	A	309	1	4,8,9	0.56	0	0,9,11	-	-
1	MSO	B	309	1	4,8,9	0.86	0	0,9,11	-	-

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	MSO	A	309	1	-	0/4/7/9	-
1	MSO	B	309	1	-	1/4/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	309	MSO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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	438/486 (90%)	1.01	80 (18%)	3 3	16, 43, 79, 93	3 (0%)
1	B	420/486 (86%)	0.94	64 (15%)	5 5	16, 43, 75, 89	4 (0%)
All	All	858/972 (88%)	0.98	144 (16%)	4 3	16, 43, 77, 93	7 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ILE	5.6
1	A	260	ALA	5.5
1	A	63	TYR	5.4
1	B	49	ALA	5.4
1	B	294	GLY	5.2
1	B	50	PRO	5.2
1	B	24	ILE	5.1
1	A	56	TYR	4.8
1	A	49	ALA	4.8
1	B	56	TYR	4.7
1	B	183	PRO	4.7
1	A	50	PRO	4.3
1	A	13	ALA	4.2
1	B	62	VAL	4.2
1	B	364	SER	4.2
1	B	52	SER	4.1
1	B	17	PRO	4.0
1	A	62	VAL	3.9
1	A	484	LEU	3.8
1	A	485	THR	3.8
1	A	16	PRO	3.8
1	B	258	TYR	3.7
1	A	185	VAL	3.7
1	A	258	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	69	GLY	3.7
1	A	14	VAL	3.7
1	B	241	PHE	3.6
1	A	10	ILE	3.6
1	A	51	GLY	3.5
1	B	217	ASN	3.5
1	A	27	GLU	3.5
1	B	244	CYS	3.5
1	B	182	ARG	3.5
1	A	256	PRO	3.4
1	A	259	LEU	3.4
1	B	53	THR	3.4
1	B	363	VAL	3.4
1	A	346	PRO	3.2
1	A	364	SER	3.2
1	A	60	GLU	3.2
1	A	182	ARG	3.2
1	B	261	ASN	3.2
1	B	54	GLU	3.1
1	A	17	PRO	3.1
1	A	53	THR	3.1
1	A	252	THR	3.1
1	B	18	HIS	3.1
1	A	294	GLY	3.1
1	B	479	LEU	3.0
1	A	262	SER	3.0
1	B	51	GLY	3.0
1	B	317[A]	ASP	3.0
1	A	483	THR	2.9
1	B	21	GLU	2.9
1	B	60	GLU	2.9
1	A	263	LEU	2.9
1	B	61	ILE	2.9
1	A	12	THR	2.9
1	A	255	LEU	2.8
1	B	454	ALA	2.8
1	A	363	VAL	2.8
1	A	452	ASP	2.8
1	A	243	GLY	2.7
1	A	417	ASN	2.7
1	A	52	SER	2.7
1	A	332	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	192	THR	2.6
1	B	251	ILE	2.6
1	B	346	PRO	2.6
1	B	260	ALA	2.6
1	A	35	ALA	2.6
1	B	48	ALA	2.6
1	A	23	ASN	2.6
1	B	20	THR	2.6
1	B	57	SER	2.6
1	A	253	ALA	2.5
1	A	422	ALA	2.5
1	A	242	ASP	2.5
1	B	58	LEU	2.5
1	A	482	ASN	2.5
1	B	473	ASP	2.5
1	B	69	GLY	2.5
1	B	192	THR	2.5
1	B	413	PHE	2.5
1	B	339	SER	2.5
1	A	365	ILE	2.5
1	A	57	SER	2.5
1	A	241	PHE	2.5
1	B	185	VAL	2.5
1	A	58	LEU	2.5
1	A	61	ILE	2.4
1	A	240	ASP	2.4
1	A	48	ALA	2.4
1	A	250	GLU	2.4
1	B	254	GLU	2.4
1	A	257	ILE	2.4
1	A	18	HIS	2.4
1	B	242	ASP	2.4
1	A	416	ARG	2.4
1	A	184	VAL	2.4
1	A	26	ASP	2.3
1	B	191	SER	2.3
1	A	187	VAL	2.3
1	B	365	ILE	2.3
1	A	296	ASN	2.3
1	B	23	ASN	2.3
1	A	181	LYS	2.3
1	B	22	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	ALA	2.3
1	B	264	ASN	2.3
1	A	486	SER	2.3
1	A	44	VAL	2.3
1	B	36	VAL	2.3
1	B	474	VAL	2.3
1	A	264	ASN	2.2
1	B	177	LEU	2.2
1	B	468	PHE	2.2
1	A	251	ILE	2.2
1	A	261	ASN	2.2
1	B	341	TRP	2.2
1	A	64	ARG	2.2
1	A	70	LEU	2.2
1	B	158	HIS	2.2
1	A	454	ALA	2.2
1	B	82	ARG	2.1
1	A	22	ASP	2.1
1	B	344	PHE	2.1
1	A	20	THR	2.1
1	A	475	LEU	2.1
1	A	479	LEU	2.1
1	B	239	THR	2.1
1	B	247	LEU	2.1
1	B	257	ILE	2.1
1	A	344	PHE	2.1
1	A	239	THR	2.1
1	A	470	ALA	2.1
1	B	259	LEU	2.1
1	A	34	ASN	2.1
1	A	59	ASP	2.1
1	B	219	ILE	2.1
1	B	475	LEU	2.0
1	B	184	VAL	2.0
1	B	162	PHE	2.0
1	A	183	PRO	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	MSO	A	309	9/10	0.90	0.17	41,41,43,44	0
1	MSO	B	309	9/10	0.92	0.18	41,42,44,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.