



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:24 PM EDT

PDB ID : 6WCS / pdb_00006wcs
Title : Crystal structure of Arabidopsis thaliana isochorismoyl-glutamate A pyruvoyl-glutamate lyase in complex with tartrate
Authors : Torrens-Spence, M.P.; Weng, J.K.
Deposited on : 2020-03-31
Resolution : 1.87 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

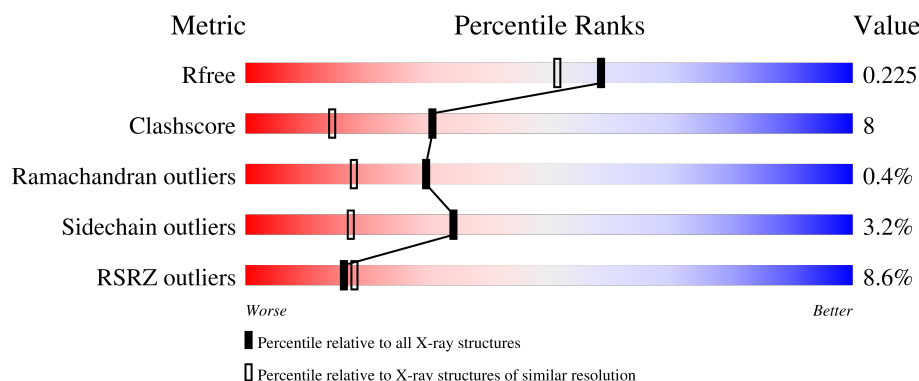
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	438	7% 80% 17% .
1	B	438	10% 72% 22% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7094 atoms, of which 4 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.

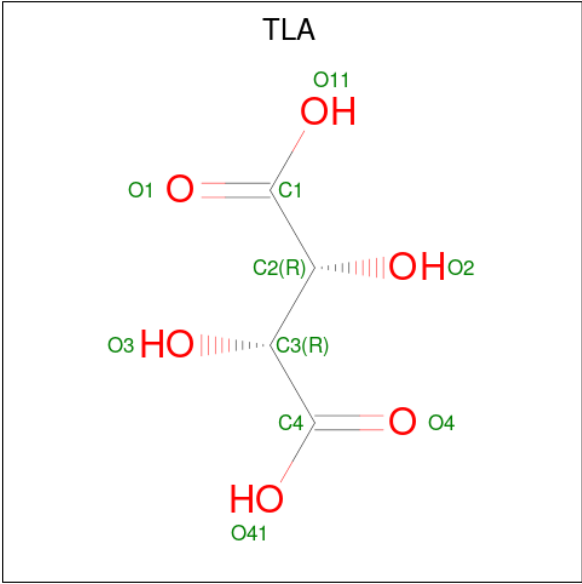
- Molecule 1 is a protein called Protein ENHANCED PSEUDOMONAS SUSCEPTIBILITY 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3451	2208	586	642	15			
1	B	421	Total	C	N	O	S	0	0	0
			3325	2130	566	615	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q9FH97
A	-2	ALA	-	expression tag	UNP Q9FH97
A	-1	HIS	-	expression tag	UNP Q9FH97
A	0	GLY	-	expression tag	UNP Q9FH97
B	-3	ALA	-	expression tag	UNP Q9FH97
B	-2	ALA	-	expression tag	UNP Q9FH97
B	-1	HIS	-	expression tag	UNP Q9FH97
B	0	GLY	-	expression tag	UNP Q9FH97

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	4	4	6		

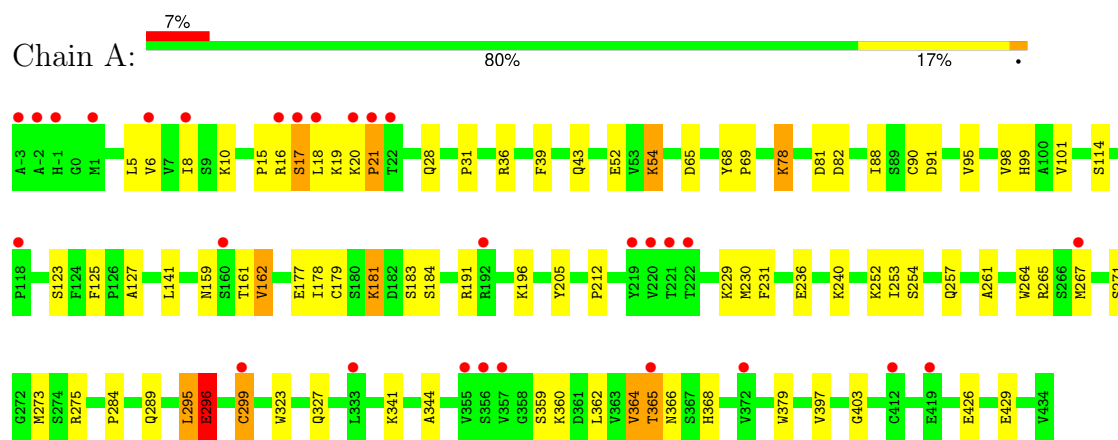
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		
3	B	107	Total	O	0	0
			107	107		

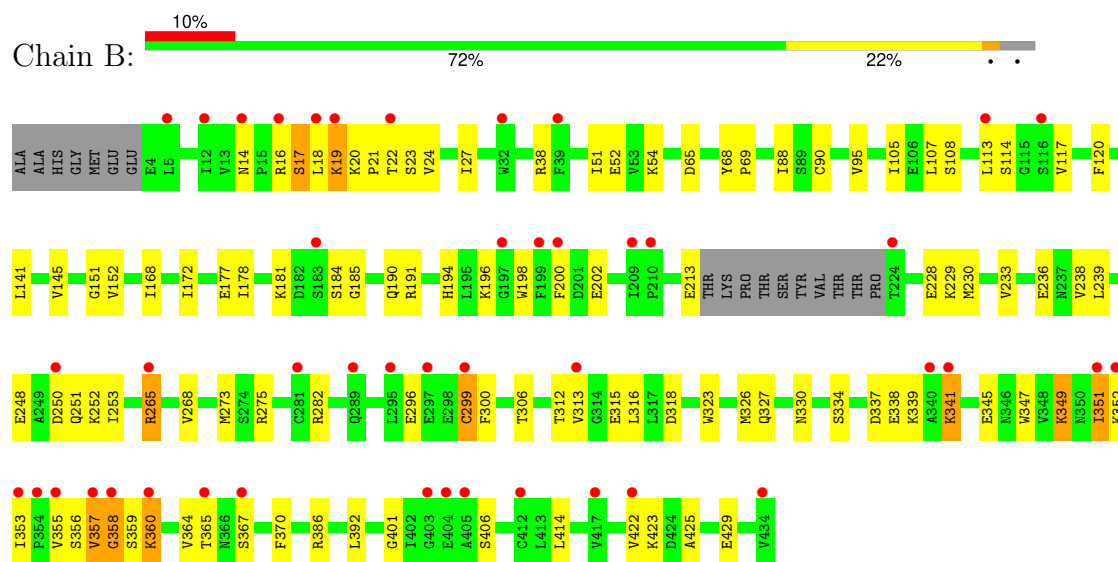
3 Residue-property plots [i](#)

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: Protein ENHANCED PSEUDOMONAS SUSCEPTIBILITY 1



• Molecule 1: Protein ENHANCED PSEUDOMONAS SUSCEPTIBILITY 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.35Å 79.43Å 194.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.52 – 1.87 73.52 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.6 (73.52-1.87) 99.9 (73.52-1.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.203 , 0.226 0.205 , 0.225	Depositor DCC
R_{free} test set	3417 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7094	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: TLA

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	0.74	25/3530 (0.7%)	0.64	8/4781 (0.2%)
1	B	0.65	4/3399 (0.1%)	0.68	3/4599 (0.1%)
All	All	0.70	29/6929 (0.4%)	0.66	11/9380 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	LYS	C-O	-7.25	1.15	1.24
1	A	364	VAL	C-O	-6.99	1.16	1.24
1	A	91	ASP	C-O	-6.97	1.14	1.24
1	A	231	PHE	C-O	-6.82	1.15	1.24
1	A	229	LYS	C-O	-6.78	1.15	1.23
1	B	364	VAL	C-O	-6.64	1.16	1.24
1	A	295	LEU	C-O	-6.41	1.15	1.23
1	B	300	PHE	C-O	-6.23	1.16	1.23
1	A	177	GLU	C-O	-6.11	1.17	1.24
1	A	179	CYS	C-O	-6.07	1.17	1.24
1	A	18	LEU	N-CA	-6.05	1.40	1.46
1	B	365	THR	C-O	-5.99	1.16	1.23
1	A	230	MET	C-O	-5.91	1.16	1.24
1	A	162	VAL	C-O	-5.91	1.18	1.24
1	A	159	ASN	C-O	-5.90	1.16	1.24
1	A	178	ILE	C-O	-5.88	1.17	1.24
1	A	296	GLU	C-O	-5.81	1.16	1.23
1	A	184	SER	C-O	-5.79	1.16	1.24
1	A	161	THR	C-O	-5.59	1.16	1.24
1	A	365	THR	C-O	-5.57	1.16	1.23
1	A	341	LYS	C-O	-5.54	1.17	1.24
1	A	90	CYS	C-O	-5.50	1.17	1.23
1	A	191	ARG	C-O	-5.47	1.16	1.23
1	A	18	LEU	CA-C	-5.39	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLU	CA-C	-5.35	1.45	1.52
1	A	366	ASN	C-O	-5.31	1.17	1.24
1	A	368	HIS	C-O	-5.15	1.17	1.24
1	A	78	LYS	C-O	-5.10	1.17	1.24
1	B	414	LEU	C-O	-5.07	1.17	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	N-CA-C	-7.75	99.02	111.04
1	A	19	LYS	N-CA-C	7.21	119.88	110.43
1	A	15	PRO	CA-C-N	-6.30	112.52	122.73
1	A	15	PRO	C-N-CA	-6.30	112.52	122.73
1	A	275	ARG	N-CA-C	6.28	119.79	111.75
1	A	114	SER	N-CA-C	6.17	119.91	112.38
1	A	183	SER	N-CA-C	6.16	119.89	112.38
1	A	21	PRO	N-CA-C	-6.07	99.97	112.47
1	B	351	ILE	CB-CA-C	6.04	121.20	111.29
1	B	185	GLY	CA-C-N	5.07	127.78	120.38
1	B	185	GLY	C-N-CA	5.07	127.78	120.38

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	3451	0	3445	44	0
1	B	3325	0	3322	69	0
2	A	10	4	4	0	0
3	A	197	0	0	1	0
3	B	107	0	0	3	0
All	All	7090	4	6771	112	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 8.

All (112) 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:358:GLY:O	1:B:392:LEU:HD11	1.79	0.82
1:B:233:VAL:HG12	1:B:238:VAL:HG23	1.63	0.80
1:B:196:LYS:HA	1:B:299:CYS:SG	2.22	0.80
1:B:17:SER:HB2	1:B:65:ASP:OD2	1.82	0.78
1:B:18:LEU:O	1:B:18:LEU:HG	1.88	0.73
1:B:425:ALA:O	1:B:429:GLU:HG2	1.88	0.73
1:B:337:ASP:OD2	1:B:341:LYS:NZ	2.22	0.72
1:A:181:LYS:N	1:A:181:LYS:HD3	2.07	0.69
1:B:265:ARG:HG2	1:B:316:LEU:HG	1.76	0.67
1:A:196:LYS:HA	1:A:299:CYS:SG	2.35	0.66
1:B:252:LYS:O	1:B:253:ILE:HD13	1.96	0.66
1:B:51:ILE:HB	1:B:152:VAL:HG11	1.79	0.64
1:A:95:VAL:HG13	1:A:141:LEU:O	1.98	0.63
1:B:38:ARG:HD2	1:B:355:VAL:HG22	1.80	0.63
1:B:95:VAL:HG13	1:B:141:LEU:O	2.00	0.61
1:B:265:ARG:HD2	1:B:316:LEU:O	2.00	0.61
1:B:14:ASN:ND2	3:B:501:HOH:O	2.21	0.61
1:A:43:GLN:NE2	1:A:127:ALA:H	1.99	0.60
1:A:10:LYS:HG2	1:A:98:VAL:HG22	1.84	0.59
1:A:5:LEU:HD22	1:A:123:SER:HB2	1.84	0.59
1:B:347:TRP:CZ2	1:B:351:ILE:HG23	2.38	0.58
1:B:323:TRP:O	1:B:327:GLN:HG2	2.03	0.58
1:B:338:GLU:H	1:B:338:GLU:CD	2.13	0.57
1:A:323:TRP:O	1:A:327:GLN:HG2	2.05	0.57
1:A:52:GLU:HB2	1:A:379:TRP:CZ2	2.41	0.56
1:B:337:ASP:CG	1:B:341:LYS:NZ	2.64	0.56
1:A:81:ASP:O	1:A:82:ASP:HB2	2.06	0.54
1:B:113:LEU:HA	3:B:508:HOH:O	2.08	0.54
1:B:251:GLN:CD	1:B:326:MET:HG2	2.32	0.54
1:A:43:GLN:NE2	1:A:125:PHE:HB3	2.23	0.53
1:A:43:GLN:HE22	1:A:127:ALA:H	1.55	0.53
1:A:236:GLU:O	1:A:240:LYS:HG3	2.09	0.52
1:B:337:ASP:OD1	1:B:341:LYS:NZ	2.42	0.52
1:A:296:GLU:N	1:A:296:GLU:OE2	2.39	0.52
1:B:252:LYS:C	1:B:253:ILE:HD13	2.34	0.52
1:A:296:GLU:H	1:A:296:GLU:CD	2.18	0.52
1:B:251:GLN:CG	1:B:326:MET:HG2	2.40	0.52
1:B:312:THR:OG1	1:B:315:GLU:HB2	2.10	0.52
1:B:114:SER:OG	1:B:229:LYS:HE2	2.10	0.51
1:B:22:THR:HG23	1:B:23:SER:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:HG23	1:B:23:SER:N	2.25	0.51
1:B:117:VAL:HG11	1:B:228:GLU:HG3	1.93	0.51
1:A:254:SER:OG	1:A:257:GLN:HG3	2.11	0.51
1:B:21:PRO:HG2	1:B:23:SER:O	2.11	0.50
1:B:24:VAL:HG13	1:B:90:CYS:O	2.11	0.50
1:A:271:SER:OG	1:A:273:MET:HG3	2.12	0.49
1:A:8:ILE:N	1:A:99:HIS:O	2.46	0.49
1:B:27:ILE:HB	1:B:88:ILE:HB	1.95	0.48
1:A:68:TYR:CG	1:A:69:PRO:HD3	2.49	0.48
1:B:251:GLN:OE1	1:B:326:MET:HG2	2.13	0.48
1:B:68:TYR:CG	1:B:69:PRO:HD3	2.49	0.48
1:A:17:SER:HB3	1:A:65:ASP:OD1	2.14	0.47
1:B:38:ARG:HH11	1:B:355:VAL:CG2	2.27	0.47
1:A:16:ARG:O	1:A:65:ASP:CB	2.62	0.47
1:B:16:ARG:NH1	1:B:184:SER:O	2.47	0.47
1:A:296:GLU:N	1:A:296:GLU:CD	2.72	0.47
1:A:365:THR:CG2	1:A:397:VAL:HG22	2.44	0.47
1:B:145:VAL:O	1:B:145:VAL:HG13	2.15	0.47
1:B:54:LYS:N	1:B:54:LYS:HD3	2.28	0.46
1:A:6:VAL:HB	1:A:101:VAL:HG13	1.98	0.46
1:A:261:ALA:O	1:A:265:ARG:HG3	2.16	0.46
1:B:360:LYS:HZ2	1:B:360:LYS:H	1.62	0.46
1:B:177:GLU:HG3	1:B:181:LYS:HE3	1.97	0.45
1:A:28:GLN:HG3	1:A:205:TYR:CD1	2.52	0.45
1:A:36:ARG:HA	1:A:39:PHE:CD2	2.52	0.45
1:A:273:MET:HG2	1:A:360:LYS:HD3	1.98	0.45
1:A:252:LYS:HZ3	1:A:253:ILE:C	2.25	0.45
1:A:273:MET:CG	1:A:360:LYS:HD3	2.47	0.45
1:A:426:GLU:O	1:A:429:GLU:HB2	2.17	0.45
1:B:19:LYS:HE2	1:B:19:LYS:HB2	1.43	0.44
1:B:107:LEU:HD21	1:B:151:GLY:HA3	1.99	0.44
1:B:168:ILE:O	1:B:172:ILE:HG12	2.17	0.44
1:B:114:SER:HA	1:B:228:GLU:O	2.16	0.44
1:A:212:PRO:O	3:A:901:HOH:O	2.21	0.44
1:A:16:ARG:O	1:A:65:ASP:HB2	2.18	0.44
1:B:349:LYS:HD3	1:B:349:LYS:HA	1.61	0.44
1:B:38:ARG:HH11	1:B:355:VAL:HG23	1.82	0.44
1:B:282:ARG:NH2	1:B:306:THR:HG21	2.33	0.44
1:A:254:SER:OG	1:A:257:GLN:CG	2.66	0.43
1:B:198:TRP:NE1	1:B:200:PHE:O	2.50	0.43
1:B:273:MET:HE3	1:B:313:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:SER:HB3	1:B:370:PHE:CE2	2.52	0.43
1:B:105:ILE:HD12	1:B:120:PHE:CD1	2.53	0.43
1:A:68:TYR:CD1	1:A:69:PRO:HD3	2.53	0.43
1:B:178:ILE:HD11	1:B:190:GLN:NE2	2.34	0.43
1:A:68:TYR:N	1:A:69:PRO:CD	2.81	0.43
1:B:273:MET:HE3	1:B:313:VAL:CG2	2.49	0.43
1:B:353:ILE:HD13	1:B:353:ILE:HG21	1.67	0.43
1:B:230:MET:HE2	1:B:386:ARG:CZ	2.48	0.43
1:A:31:PRO:HG2	1:A:344:ALA:HB1	2.00	0.43
1:A:267:MET:SD	1:A:362:LEU:HD13	2.59	0.43
1:A:403:GLY:HA3	1:B:108:SER:OG	2.18	0.43
1:B:68:TYR:CD1	1:B:69:PRO:HD3	2.54	0.42
1:B:202:GLU:OE1	1:B:345:GLU:OE1	2.37	0.42
1:B:330:ASN:O	1:B:334:SER:OG	2.31	0.42
1:A:289:GLN:NE2	1:A:295:LEU:O	2.52	0.42
1:A:88:ILE:HD13	1:A:162:VAL:HG23	2.01	0.42
1:B:228:GLU:O	1:B:229:LYS:HG2	2.19	0.42
1:B:248:GLU:CD	3:B:502:HOH:O	2.61	0.42
1:A:20:LYS:HA	1:A:21:PRO:HD3	1.72	0.42
1:A:284:PRO:HD3	1:A:364:VAL:O	2.20	0.42
1:B:296:GLU:O	1:B:299:CYS:HB2	2.20	0.42
1:B:191:ARG:NH1	1:B:194:HIS:NE2	2.68	0.41
1:B:334:SER:O	1:B:339:LYS:HD3	2.20	0.41
1:B:401:GLY:HA3	1:B:406:SER:OG	2.20	0.41
1:B:347:TRP:CH2	1:B:351:ILE:HG23	2.54	0.41
1:B:239:LEU:N	1:B:239:LEU:HD23	2.35	0.41
1:B:275:ARG:NH1	1:B:318:ASP:OD2	2.42	0.41
1:B:68:TYR:N	1:B:69:PRO:CD	2.84	0.41
1:B:268:VAL:HG21	1:B:316:LEU:CD2	2.49	0.41
1:A:271:SER:OG	1:A:273:MET:HE2	2.21	0.41
1:A:264:TRP:HB2	1:A:362:LEU:HD22	2.02	0.41

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	436/438 (100%)	426 (98%)	9 (2%)	1 (0%)	43	34
1	B	417/438 (95%)	401 (96%)	14 (3%)	2 (0%)	24	13
All	All	853/876 (97%)	827 (97%)	23 (3%)	3 (0%)	30	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	LYS
1	B	357	VAL
1	B	358	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	381/381 (100%)	375 (98%)	6 (2%)	55	43
1	B	367/381 (96%)	349 (95%)	18 (5%)	22	7
All	All	748/762 (98%)	724 (97%)	24 (3%)	34	17

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

Mol	Chain	Res	Type
1	A	17	SER
1	A	54	LYS
1	A	78	LYS
1	A	296	GLU
1	A	299	CYS
1	A	359	SER
1	B	17	SER
1	B	19	LYS
1	B	20	LYS
1	B	52	GLU

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Mol	Chain	Res	Type
1	B	213	GLU
1	B	236	GLU
1	B	250	ASP
1	B	265	ARG
1	B	299	CYS
1	B	341	LYS
1	B	349	LYS
1	B	352	LYS
1	B	356	SER
1	B	357	VAL
1	B	359	SER
1	B	360	LYS
1	B	422	VAL
1	B	423	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	43	GLN
1	A	49	HIS
1	A	55	GLN
1	A	132	ASN
1	A	173	ASN
1	A	280	HIS
1	A	375	ASN
1	B	14	ASN
1	B	49	HIS
1	B	187	GLN
1	B	190	GLN
1	B	289	GLN
1	B	346	ASN
1	B	350	ASN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	TLA	A	801	-	9,9,9	1.05	0	12,12,12	1.75	6 (50%)

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	TLA	A	801	-	-	4/12/12/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	TLA	O41-C4-C3	2.55	120.41	113.31
2	A	801	TLA	O11-C1-C2	2.39	119.94	113.31
2	A	801	TLA	C3-C2-C1	2.37	115.07	109.82
2	A	801	TLA	O41-C4-O4	-2.05	119.42	124.08
2	A	801	TLA	O11-C1-O1	-2.03	119.48	124.08
2	A	801	TLA	O2-C2-C3	-2.00	106.09	110.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	TLA	O1-C1-C2-C3
2	A	801	TLA	O11-C1-C2-C3
2	A	801	TLA	O1-C1-C2-O2
2	A	801	TLA	O11-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	438/438 (100%)	0.38	29 (6%) 24 27	24, 39, 66, 137	0
1	B	421/438 (96%)	0.78	45 (10%) 11 13	30, 51, 88, 117	0
All	All	859/876 (98%)	0.57	74 (8%) 16 18	24, 44, 82, 137	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	VAL	5.3
1	A	219	TYR	4.4
1	B	224	THR	3.9
1	B	18	LEU	3.7
1	A	-3	ALA	3.7
1	B	22	THR	3.6
1	B	197	GLY	3.6
1	B	434	VAL	3.5
1	B	299	CYS	3.4
1	B	354	PRO	3.4
1	B	404	GLU	3.4
1	B	200	PHE	3.3
1	B	358	GLY	3.3
1	B	265	ARG	3.2
1	B	32	TRP	3.1
1	B	295	LEU	3.1
1	A	222	THR	3.0
1	B	353	ILE	3.0
1	B	403	GLY	3.0
1	A	355	VAL	3.0
1	B	210	PRO	2.9
1	A	220	VAL	2.9
1	A	365	THR	2.9
1	B	12	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	14	ASN	2.8
1	B	365	THR	2.8
1	B	199	PHE	2.6
1	A	299	CYS	2.5
1	A	18	LEU	2.5
1	A	8	ILE	2.5
1	A	-2	ALA	2.5
1	B	250	ASP	2.5
1	B	360	LYS	2.4
1	A	267	MET	2.4
1	A	16	ARG	2.4
1	B	209	ILE	2.4
1	B	340	ALA	2.4
1	B	422	VAL	2.4
1	A	412	CYS	2.4
1	B	355	VAL	2.3
1	B	405	ALA	2.3
1	B	352	LYS	2.3
1	A	21	PRO	2.3
1	A	192	ARG	2.3
1	A	6	VAL	2.3
1	A	20	LYS	2.3
1	A	118	PRO	2.2
1	B	367	SER	2.2
1	B	289	GLN	2.2
1	B	313	VAL	2.2
1	A	-1	HIS	2.2
1	B	351	ILE	2.2
1	A	419	GLU	2.2
1	B	412	CYS	2.2
1	B	113	LEU	2.2
1	A	160	SER	2.2
1	B	116	SER	2.2
1	B	19	LYS	2.2
1	A	221	THR	2.2
1	B	5	LEU	2.2
1	A	1	MET	2.1
1	B	297	GLU	2.1
1	A	17	SER	2.1
1	B	16	ARG	2.1
1	A	372	VAL	2.1
1	B	417	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	LEU	2.1
1	B	183	SER	2.1
1	A	357	VAL	2.1
1	A	356	SER	2.0
1	B	281	CYS	2.0
1	B	341	LYS	2.0
1	B	39	PHE	2.0
1	A	22	THR	2.0

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 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($\text{\AA}^2$)	Q<0.9
2	TLA	A	801	10/10	0.69	0.17	57,70,84,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.