



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2021 – 08:03 PM EDT

PDB ID : 6WCS
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
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) : 2.22

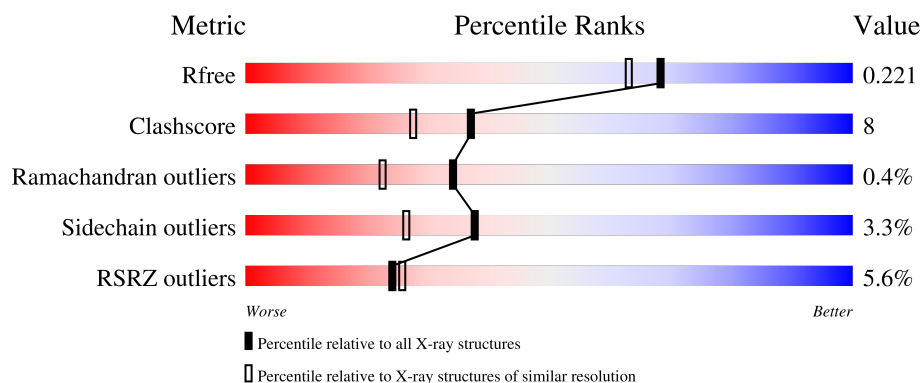
1 Overall quality at a glance

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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	438	<div> <div>8%</div> <div>74%</div> <div>20%</div> <div>.</div> <div>.</div> </div>

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.

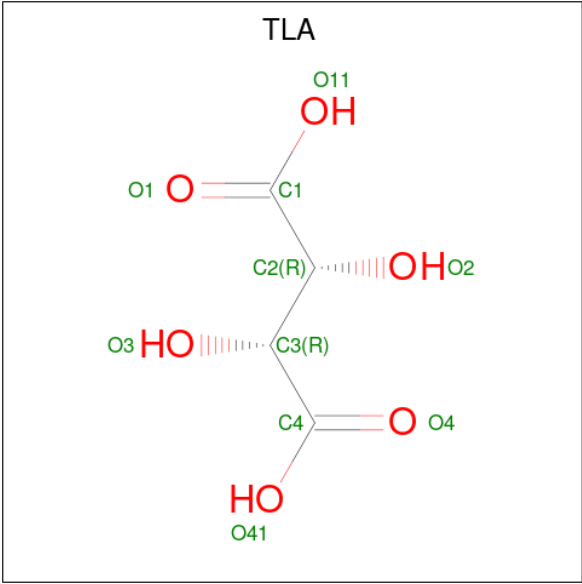
- Molecule 1 is a protein called Protein ENHANCED PSEUDOMONAS SUSCEPTIBILITY 1.

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 (three-letter code: TLA) (formula: C₄H₆O₆).



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

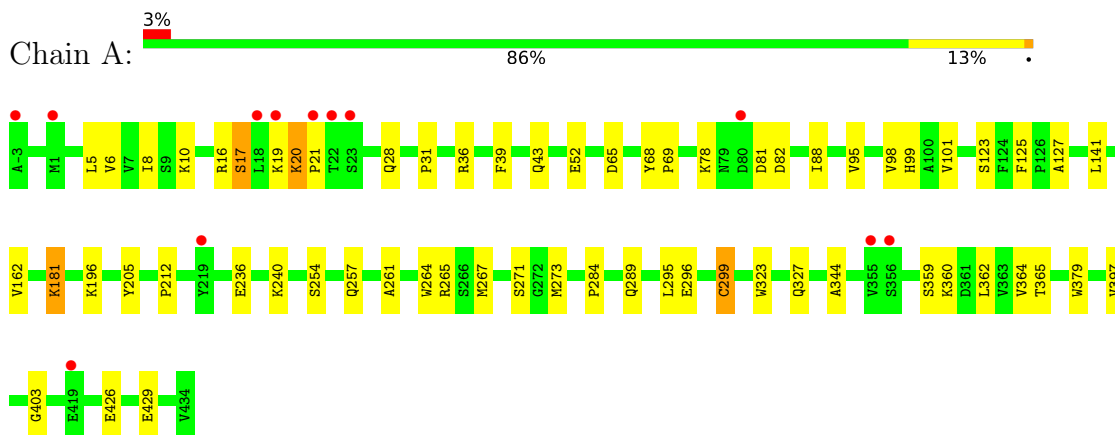
- Molecule 3 is water.

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

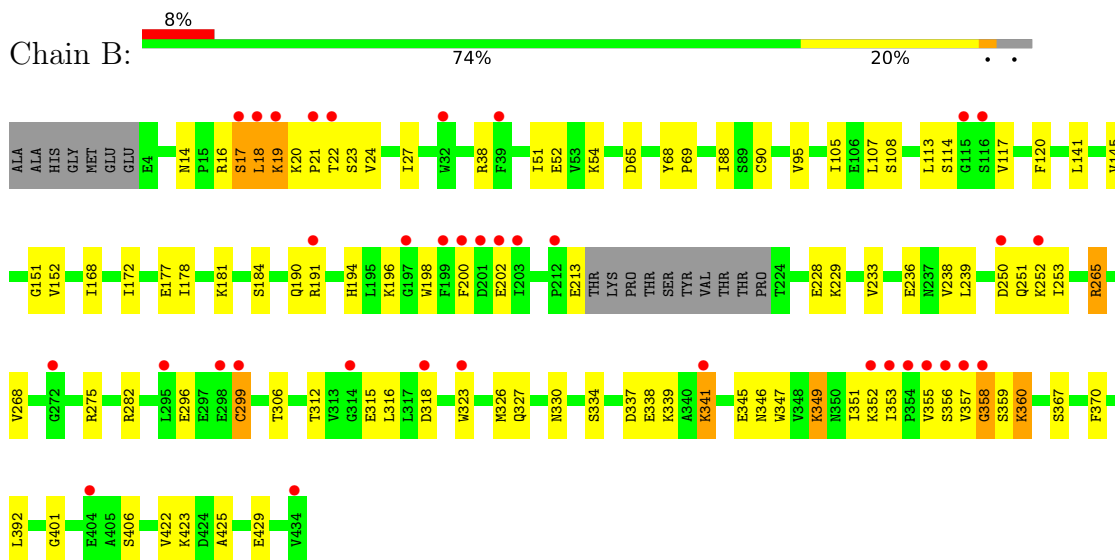
3 Residue-property plots [i](#)

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 97.11 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.6 (73.52-1.87) 99.6 (97.11-1.87)	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 0.202 , 0.221	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 , 44.4	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	0.56	0/3530	0.55	0/4781
1	B	0.50	0/3399	0.57	0/4599
All	All	0.53	0/6929	0.56	0/9380

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

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	42	0
1	B	3325	0	3322	65	0
2	A	10	4	4	0	0
3	A	197	0	0	1	0
3	B	107	0	0	2	0
All	All	7090	4	6771	106	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 (106) 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: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: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: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:338:GLU:H	1:B:338:GLU:CD	2.13	0.52
1:A:296:GLU:N	1:A:296:GLU:OE2	2.39	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
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:337:ASP:CG	1:B:341:LYS:NZ	2.64	0.51
1:B:21:PRO:HG2	1:B:23:SER:O	2.11	0.50
1:B:337:ASP:OD1	1:B:341:LYS:NZ	2.42	0.50
1:B:24:VAL:HG13	1:B:90:CYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:SER:OG	1:A:273:MET:HG3	2.12	0.49
1:B:251:GLN:CD	1:B:326:MET:HG2	2.32	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:252:LYS:C	1:B:253:ILE:HD13	2.34	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:H	1:A:296:GLU:CD	2.18	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	1.64	0.45
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ILE:HD13	1:B:353:ILE:HG21	1.67	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:A:296:GLU:N	1:A:296:GLU:CD	2.72	0.42
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: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:264:TRP:HB2	1:A:362:LEU:HD22	2.02	0.41

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	436/438 (100%)	426 (98%)	9 (2%)	1 (0%)	47	37
1	B	417/438 (95%)	401 (96%)	14 (3%)	2 (0%)	29	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	853/876 (97%)	827 (97%)	23 (3%)	3 (0%)	34	22

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%)	62	56
1	B	367/381 (96%)	348 (95%)	19 (5%)	23	12
All	All	748/762 (98%)	723 (97%)	25 (3%)	38	26

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	19	LYS
1	A	20	LYS
1	A	78	LYS
1	A	299	CYS
1	A	359	SER
1	B	17	SER
1	B	18	LEU
1	B	19	LYS
1	B	20	LYS
1	B	52	GLU
1	B	213	GLU
1	B	236	GLU
1	B	250	ASP
1	B	265	ARG

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Mol	Chain	Res	Type
1	B	299	CYS
1	B	341	LYS
1	B	346	ASN
1	B	349	LYS
1	B	352	LYS
1	B	356	SER
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	55	GLN
1	A	173	ASN
1	A	375	ASN
1	B	173	ASN
1	B	187	GLN
1	B	190	GLN
1	B	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	3,9,9	1.02	0	6,12,12	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	A	801	-	-	0/4/12/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	0.25	12 (2%) 54 56	24, 39, 66, 137	0
1	B	421/438 (96%)	0.50	36 (8%) 10 11	30, 51, 88, 117	0
All	All	859/876 (98%)	0.37	48 (5%) 24 26	24, 44, 82, 137	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	VAL	10.5
1	B	352	LYS	5.6
1	A	-3	ALA	5.3
1	A	219	TYR	5.1
1	B	355	VAL	5.1
1	A	355	VAL	4.8
1	B	22	THR	4.6
1	A	18	LEU	4.2
1	B	18	LEU	3.8
1	B	295	LEU	3.8
1	B	212	PRO	3.7
1	B	404	GLU	3.6
1	B	199	PHE	3.5
1	B	39	PHE	3.5
1	B	356	SER	3.4
1	A	22	THR	3.3
1	B	19	LYS	3.1
1	B	202	GLU	3.1
1	B	314	GLY	3.1
1	B	250	ASP	2.9
1	B	32	TRP	2.8
1	B	191	ARG	2.7
1	B	353	ILE	2.7
1	B	358	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	19	LYS	2.7
1	A	23	SER	2.7
1	B	299	CYS	2.6
1	A	21	PRO	2.6
1	B	200	PHE	2.6
1	B	318	ASP	2.5
1	B	252	LYS	2.4
1	B	341	LYS	2.4
1	B	354	PRO	2.4
1	A	356	SER	2.4
1	B	17	SER	2.3
1	B	116	SER	2.3
1	B	272	GLY	2.3
1	B	434	VAL	2.2
1	B	197	GLY	2.2
1	B	115	GLY	2.2
1	A	1	MET	2.1
1	B	323	TRP	2.1
1	B	21	PRO	2.1
1	A	80	ASP	2.1
1	A	419	GLU	2.1
1	B	298	GLU	2.1
1	B	203	ILE	2.1
1	B	201	ASP	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 monosaccharides 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(\AA^2)	Q<0.9
2	TLA	A	801	10/10	0.66	0.27	57,70,84,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.