



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:46 PM UTC

PDB ID : 2GPT / pdb_00002gpt
Title : Crystal structure of Arabidopsis Dehydroquinate dehydratase-shikimate dehydrogenase in complex with tartrate and shikimate
Authors : Singh, S.A.; Christendat, D.
Deposited on : 2006-04-18
Resolution : 1.95 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

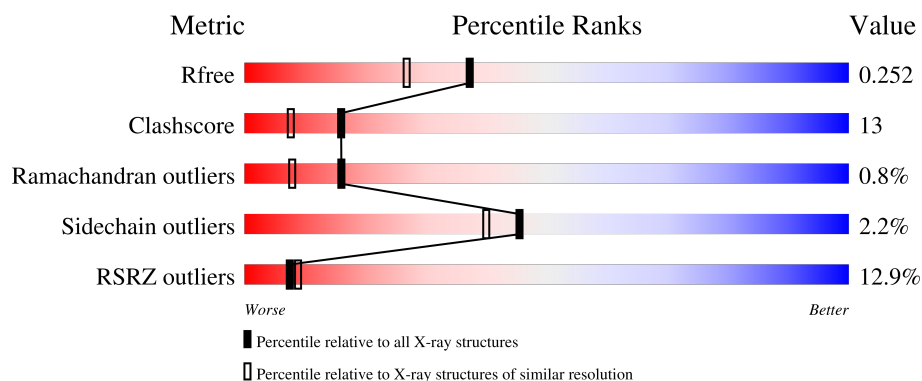
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	523	12% 71% 22% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4143 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.

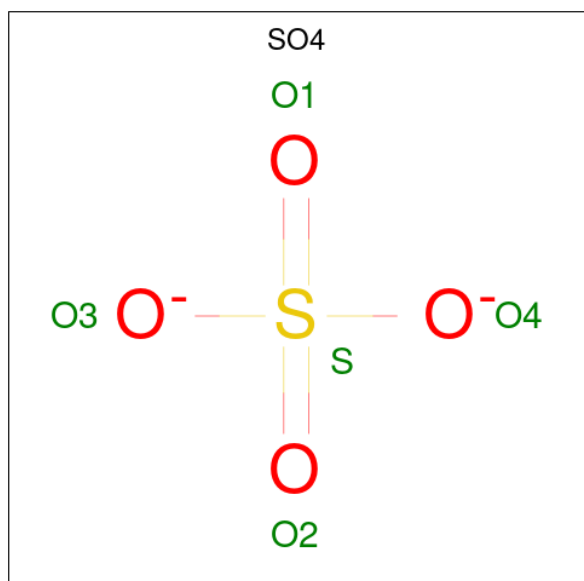
- Molecule 1 is a protein called 3-dehydroquinate dehydratase/ shikimate 5-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3840	2441	642	740	17	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

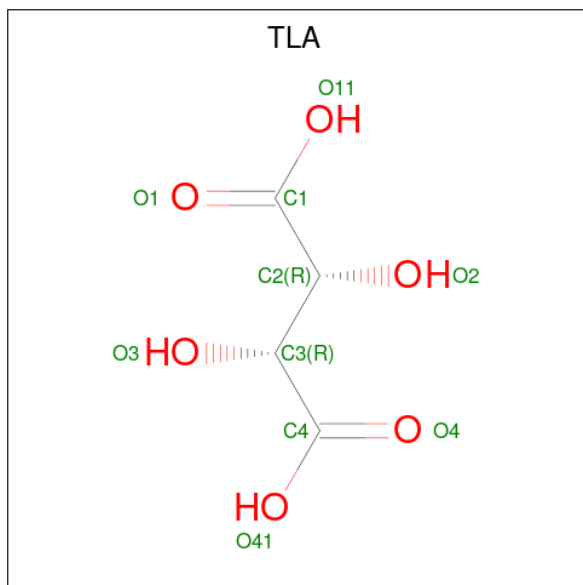
Chain	Residue	Modelled	Actual	Comment	Reference
A	604	GLY	-	cloning artifact	UNP Q9SQT8
A	605	SER	-	cloning artifact	UNP Q9SQT8
A	606	ARG	-	cloning artifact	UNP Q9SQT8
A	607	GLU	-	cloning artifact	UNP Q9SQT8
A	608	ASN	-	cloning artifact	UNP Q9SQT8
A	609	LEU	-	cloning artifact	UNP Q9SQT8
A	610	TYR	-	cloning artifact	UNP Q9SQT8
A	611	PHE	-	cloning artifact	UNP Q9SQT8
A	612	GLN	-	cloning artifact	UNP Q9SQT8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



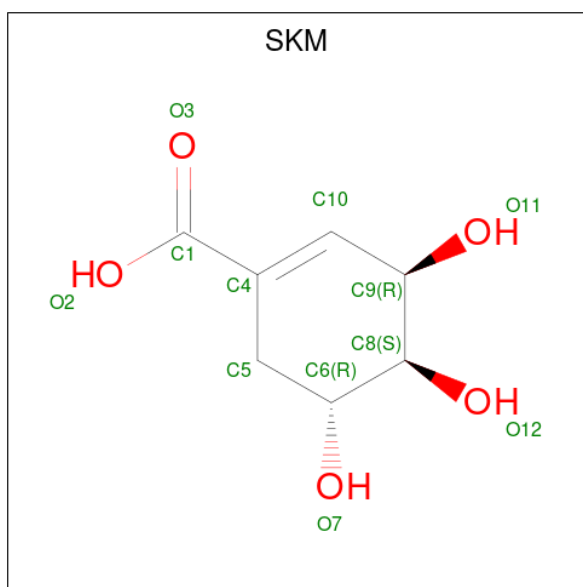
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is (3R,4S,5R)-3,4,5-TRIHIDROXYCYCLOHEX-1-ENE-1-CARBOXYLIC ACID (CCD ID: SKM) (formula: C₇H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	7	5		

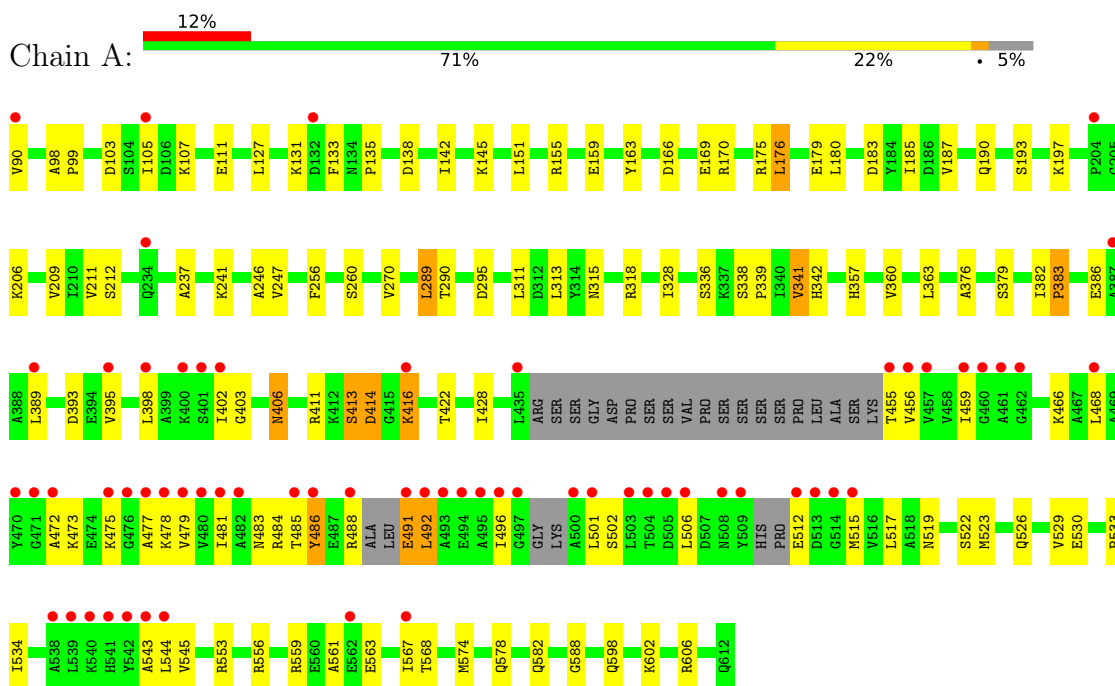
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	271	Total	O	0	0
			271	271		

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: 3-dehydroquinate dehydratase/ shikimate 5-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.93Å 96.93Å 116.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.46 – 1.95 28.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.4 (28.46-1.95) 66.8 (28.46-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.256 0.219 , 0.252	Depositor DCC
R_{free} test set	936 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4143	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: SKM, SO4, 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	0.37	0/3907	0.90	13/5281 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ALA	N-CA-C	5.72	119.99	112.89
1	A	336	SER	N-CA-C	5.57	118.31	110.23
1	A	529	VAL	N-CA-C	5.54	118.01	111.09
1	A	360	VAL	N-CA-C	5.49	115.76	107.80
1	A	379	SER	N-CA-C	-5.36	101.43	109.95
1	A	145	LYS	N-CA-C	5.30	119.01	112.54
1	A	155	ARG	CA-C-N	5.28	125.74	120.14
1	A	155	ARG	C-N-CA	5.28	125.74	120.14
1	A	311	LEU	N-CA-C	5.21	116.77	111.14
1	A	588	GLY	N-CA-C	-5.16	108.12	115.30
1	A	247	VAL	N-CA-C	-5.12	105.13	112.35
1	A	212	SER	N-CA-C	5.11	117.92	109.85
1	A	341	VAL	N-CA-C	5.02	115.24	110.42

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	3840	0	3861	102	0
2	A	10	0	0	1	0
3	A	10	0	4	0	0
4	A	12	0	9	1	0
5	A	271	0	0	10	0
All	All	4143	0	3874	102	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 (102) 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:103:ASP:HB2	1:A:131:LYS:HG2	1.47	0.96
1:A:481:ILE:HG13	1:A:492:LEU:HD12	1.53	0.90
1:A:411:ARG:HH21	1:A:416:LYS:HD2	1.38	0.89
1:A:411:ARG:NH2	1:A:416:LYS:HD2	1.88	0.88
1:A:545:VAL:HG11	1:A:561:ALA:HB1	1.59	0.84
1:A:456:VAL:HB	1:A:479:VAL:HG12	1.63	0.80
1:A:428:ILE:HG21	1:A:475:LYS:HD2	1.63	0.80
1:A:105:ILE:HD11	1:A:142:ILE:HG13	1.69	0.75
1:A:473:LYS:HD2	1:A:496:ILE:HB	1.70	0.73
1:A:545:VAL:HG11	1:A:561:ALA:CB	2.19	0.71
1:A:416:LYS:NZ	1:A:416:LYS:HB3	2.07	0.69
1:A:105:ILE:HG22	5:A:5247:HOH:O	1.93	0.68
1:A:543:ALA:O	1:A:567:ILE:HG22	1.92	0.68
1:A:393:ASP:OD2	1:A:416:LYS:HB2	1.95	0.67
1:A:556:ARG:HG3	1:A:559:ARG:NH2	2.10	0.67
1:A:206:LYS:HG3	5:A:5199:HOH:O	1.94	0.66
1:A:456:VAL:HB	1:A:479:VAL:CG1	2.27	0.64
1:A:175:ARG:O	1:A:179:GLU:HG2	1.98	0.64
1:A:166:ASP:OD2	1:A:169:GLU:HG3	1.98	0.63
1:A:501:LEU:HD23	1:A:502:SER:N	2.14	0.62
1:A:544:LEU:HD23	1:A:545:VAL:N	2.14	0.62
1:A:386:GLU:HG3	1:A:466:LYS:HZ2	1.66	0.61
1:A:105:ILE:HD11	1:A:142:ILE:CG1	2.31	0.60
1:A:459:ILE:HD11	1:A:517:LEU:HD11	1.83	0.60
1:A:473:LYS:HG3	1:A:478:LYS:NZ	2.16	0.60
1:A:559:ARG:O	1:A:563:GLU:HG3	2.02	0.60
1:A:473:LYS:HG3	1:A:478:LYS:HZ3	1.68	0.57
1:A:523:MET:HE3	1:A:533:PRO:HB3	1.85	0.57
1:A:506:LEU:HG	1:A:534:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:HE21	1:A:190:GLN:HA	1.69	0.57
1:A:414:ASP:OD1	1:A:416:LYS:HG2	2.06	0.56
1:A:406:ASN:HD21	1:A:422:THR:H	1.54	0.56
1:A:414:ASP:OD2	1:A:416:LYS:HE2	2.05	0.56
1:A:416:LYS:HB3	1:A:416:LYS:HZ3	1.70	0.55
1:A:598:GLN:NE2	5:A:5139:HOH:O	2.39	0.54
1:A:363:LEU:C	1:A:363:LEU:HD13	2.33	0.54
1:A:389:LEU:HD22	1:A:403:GLY:C	2.33	0.54
1:A:159:GLU:O	1:A:159:GLU:HG3	2.10	0.52
1:A:185:ILE:HD11	1:A:209:VAL:HG13	1.91	0.52
1:A:211:VAL:CG2	1:A:237:ALA:HB2	2.39	0.52
1:A:246:ALA:HB2	1:A:270:VAL:CG1	2.39	0.52
1:A:183:ASP:HA	5:A:5199:HOH:O	2.09	0.52
1:A:526:GLN:NE2	5:A:5056:HOH:O	2.43	0.51
1:A:289:LEU:HD23	1:A:290:THR:N	2.26	0.51
1:A:544:LEU:HD23	1:A:544:LEU:C	2.36	0.50
1:A:468:LEU:O	1:A:468:LEU:HD23	2.11	0.50
1:A:185:ILE:HD12	1:A:185:ILE:C	2.37	0.50
1:A:406:ASN:ND2	1:A:422:THR:H	2.10	0.50
1:A:339:PRO:HG2	1:A:357:HIS:CE1	2.46	0.50
1:A:241:LYS:HE3	5:A:5019:HOH:O	2.12	0.49
1:A:574:MET:SD	1:A:574:MET:C	2.96	0.48
1:A:578:GLN:O	1:A:582:GLN:HG3	2.12	0.48
1:A:606:ARG:HH11	1:A:606:ARG:HG3	1.78	0.48
1:A:398:LEU:O	1:A:402:ILE:HG13	2.14	0.48
1:A:105:ILE:HD13	1:A:138:ASP:HB3	1.96	0.48
1:A:484:ARG:NH1	1:A:484:ARG:HB3	2.29	0.48
1:A:328:ILE:HD13	4:A:4733:SKM:H51	1.95	0.48
1:A:606:ARG:HG3	1:A:606:ARG:NH1	2.29	0.47
1:A:315:ASN:HB3	1:A:318:ARG:HD3	1.97	0.47
1:A:406:ASN:ND2	1:A:406:ASN:C	2.72	0.47
1:A:491:GLU:N	1:A:491:GLU:OE1	2.48	0.47
1:A:90:VAL:HB	5:A:5009:HOH:O	2.14	0.47
1:A:313:LEU:O	1:A:313:LEU:HD23	2.15	0.47
1:A:289:LEU:HD23	1:A:289:LEU:C	2.40	0.46
1:A:246:ALA:HB2	1:A:270:VAL:HG12	1.97	0.46
1:A:163:TYR:CD2	1:A:170:ARG:HD3	2.50	0.46
1:A:383:PRO:HA	2:A:1402:SO4:O2	2.16	0.46
1:A:382:ILE:HD12	1:A:522:SER:OG	2.15	0.46
1:A:501:LEU:HD23	1:A:501:LEU:C	2.41	0.45
1:A:553:ARG:HD2	5:A:5251:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ILE:HG12	1:A:568:THR:N	2.31	0.45
1:A:483:ASN:HD22	1:A:488:ARG:HB2	1.82	0.45
1:A:411:ARG:HH21	1:A:416:LYS:CD	2.17	0.44
1:A:295:ASP:C	1:A:295:ASP:OD2	2.61	0.44
1:A:501:LEU:HD23	1:A:502:SER:C	2.43	0.44
1:A:459:ILE:HB	1:A:519:ASN:HA	2.00	0.43
1:A:544:LEU:HG	1:A:567:ILE:HG23	2.00	0.43
1:A:211:VAL:HG21	1:A:237:ALA:HB2	2.00	0.43
1:A:341:VAL:HG23	1:A:342:HIS:N	2.34	0.43
1:A:598:GLN:HE21	1:A:602:LYS:HE3	1.84	0.42
1:A:98:ALA:HA	1:A:99:PRO:HD3	1.83	0.42
1:A:313:LEU:HD23	1:A:313:LEU:C	2.44	0.42
1:A:501:LEU:HD23	1:A:502:SER:O	2.19	0.42
1:A:512:GLU:HB2	1:A:515:MET:CG	2.50	0.42
1:A:107:LYS:O	1:A:111:GLU:HG3	2.20	0.42
1:A:472:ALA:CB	1:A:479:VAL:HG11	2.50	0.42
1:A:193:SER:O	1:A:197:LYS:HG3	2.20	0.41
1:A:256:PHE:O	1:A:260:SER:HB3	2.20	0.41
1:A:338:SER:N	1:A:339:PRO:CD	2.83	0.41
1:A:176:LEU:HD22	1:A:180:LEU:CD1	2.51	0.41
1:A:530:GLU:HA	1:A:530:GLU:OE2	2.20	0.41
1:A:187:VAL:O	1:A:211:VAL:HA	2.20	0.41
1:A:338:SER:HB2	1:A:339:PRO:HD3	2.02	0.41
1:A:131:LYS:HE2	5:A:5154:HOH:O	2.20	0.41
1:A:483:ASN:ND2	1:A:488:ARG:HB2	2.35	0.41
1:A:598:GLN:NE2	1:A:602:LYS:NZ	2.68	0.41
1:A:389:LEU:HD11	1:A:395:VAL:HG11	2.02	0.40
1:A:455:THR:O	1:A:455:THR:HG23	2.19	0.40
1:A:485:THR:O	1:A:486:TYR:C	2.65	0.40
1:A:411:ARG:HG2	1:A:413:SER:HB2	2.03	0.40
1:A:512:GLU:N	5:A:5257:HOH:O	2.54	0.40
1:A:127:LEU:HD22	1:A:133:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	488/523 (93%)	465 (95%)	19 (4%)	4 (1%)	16 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	SER
1	A	477	ALA
1	A	135	PRO
1	A	486	TYR

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	418/439 (95%)	409 (98%)	9 (2%)	45 40

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	176	LEU
1	A	289	LEU
1	A	383	PRO
1	A	406	ASN
1	A	414	ASP
1	A	416	LYS
1	A	491	GLU
1	A	492	LEU

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	92	ASN
1	A	190	GLN
1	A	233	GLN
1	A	263	GLN
1	A	315	ASN
1	A	344	GLN
1	A	368	GLN
1	A	406	ASN
1	A	483	ASN
1	A	526	GLN
1	A	598	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1402	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	A	1403	-	4,4,4	0.38	0	6,6,6	0.08	0
4	SKM	A	4733	-	12,12,12	1.20	2 (16%)	16,17,17	0.80	0
3	TLA	A	4988	-	9,9,9	0.86	0	12,12,12	1.23	2 (16%)

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
4	SKM	A	4733	-	-	0/4/20/20	0/1/1/1
3	TLA	A	4988	-	-	0/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4733	SKM	C8-C9	2.53	1.57	1.52
4	A	4733	SKM	C6-C8	2.34	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4988	TLA	O11-C1-C2	2.32	119.77	113.31
3	A	4988	TLA	O41-C4-C3	2.20	119.42	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1402	SO4	1	0
4	A	4733	SKM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	498/523 (95%)	0.65	64 (12%) 7 9	19, 33, 73, 93	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	9.0
1	A	479	VAL	6.3
1	A	500	ALA	6.3
1	A	477	ALA	6.1
1	A	514	GLY	6.0
1	A	501	LEU	6.0
1	A	509	TYR	5.9
1	A	492	LEU	5.8
1	A	493	ALA	5.2
1	A	496	ILE	4.9
1	A	503	LEU	4.9
1	A	513	ASP	4.9
1	A	504	THR	4.8
1	A	506	LEU	4.6
1	A	539	LEU	4.4
1	A	478	LYS	4.1
1	A	485	THR	3.9
1	A	476	GLY	3.9
1	A	475	LYS	3.9
1	A	540	LYS	3.9
1	A	486	TYR	3.8
1	A	481	ILE	3.8
1	A	435	LEU	3.7
1	A	472	ALA	3.7
1	A	455	THR	3.6
1	A	495	ALA	3.5
1	A	470	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	389	LEU	3.2
1	A	497	GLY	3.1
1	A	567	ILE	3.1
1	A	387	ALA	3.0
1	A	401	SER	3.0
1	A	402	ILE	2.9
1	A	480	VAL	2.9
1	A	541	HIS	2.9
1	A	471	GLY	2.9
1	A	515	MET	2.8
1	A	456	VAL	2.7
1	A	491	GLU	2.7
1	A	543	ALA	2.6
1	A	395	VAL	2.6
1	A	505	ASP	2.6
1	A	562	GLU	2.6
1	A	400	LYS	2.6
1	A	508	ASN	2.5
1	A	488	ARG	2.5
1	A	457	VAL	2.5
1	A	494	GLU	2.4
1	A	512	GLU	2.4
1	A	132	ASP	2.4
1	A	542	TYR	2.3
1	A	398	LEU	2.3
1	A	538	ALA	2.2
1	A	105	ILE	2.2
1	A	460	GLY	2.2
1	A	462	GLY	2.2
1	A	468	LEU	2.2
1	A	482	ALA	2.1
1	A	459	ILE	2.1
1	A	204	PRO	2.1
1	A	544	LEU	2.1
1	A	234	GLN	2.0
1	A	461	ALA	2.0
1	A	416	LYS	2.0

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

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	SO4	A	1403	5/5	0.80	0.23	53,53,55,55	5
3	TLA	A	4988	10/10	0.94	0.07	33,39,45,46	0
4	SKM	A	4733	12/12	0.94	0.07	25,27,33,36	0
2	SO4	A	1402	5/5	0.95	0.13	23,24,27,28	5

6.5 Other polymers [i](#)

There are no such residues in this entry.