Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 08:34 AM EST

PDB ID	:	2O7S
Title	:	Crystal Structure of the A. thaliana DHQ-dehydroshikimate-SDH-shikimate-NADP(H)
Authors	:	Christendat, D.; Singh, S.A.
Deposited on	:	2006-12-11
Resolution	:	1.78 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:

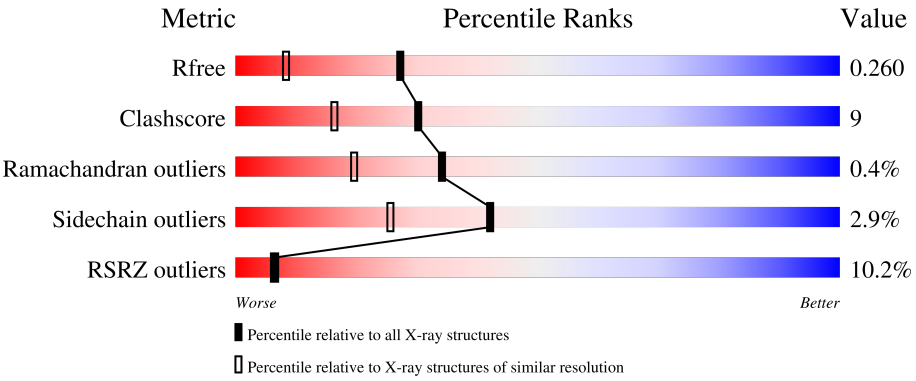
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	10% 80% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHK	A	4733	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DHK	A	9241[A]	X	-	-	-
5	NAP	A	1411	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4150 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.

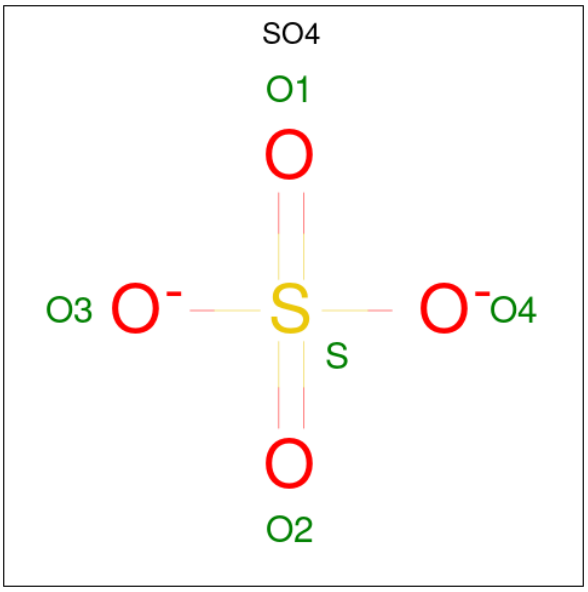
- Molecule 1 is a protein called Bifunctional 3-dehydroquinate dehydratase/shikimate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	3859	2452	645	745	17	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

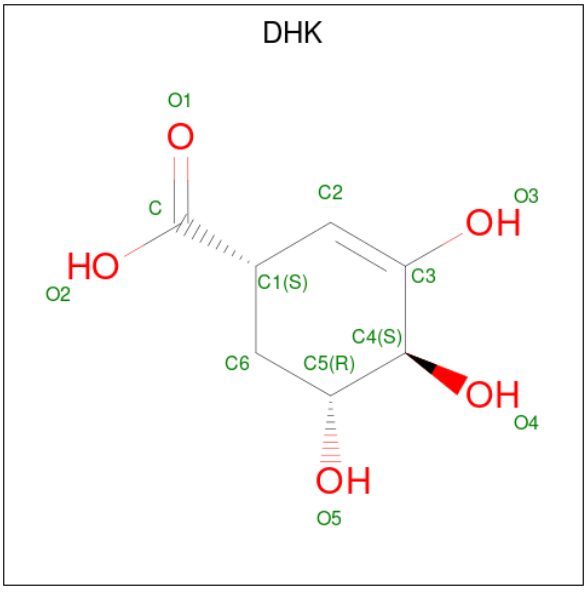
Chain	Residue	Modelled	Actual	Comment	Reference
A	391	CSO	CYS	modified residue	UNP Q9SQT8
A	424	CSO	CYS	modified residue	UNP Q9SQT8
A	604	GLY	-	expression tag	UNP Q9SQT8
A	605	SER	-	expression tag	UNP Q9SQT8
A	606	ARG	-	expression tag	UNP Q9SQT8
A	607	GLU	-	expression tag	UNP Q9SQT8
A	608	ASN	-	expression tag	UNP Q9SQT8
A	609	LEU	-	expression tag	UNP Q9SQT8
A	610	TYR	-	expression tag	UNP Q9SQT8
A	611	PHE	-	expression tag	UNP Q9SQT8
A	612	GLN	-	expression tag	UNP Q9SQT8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



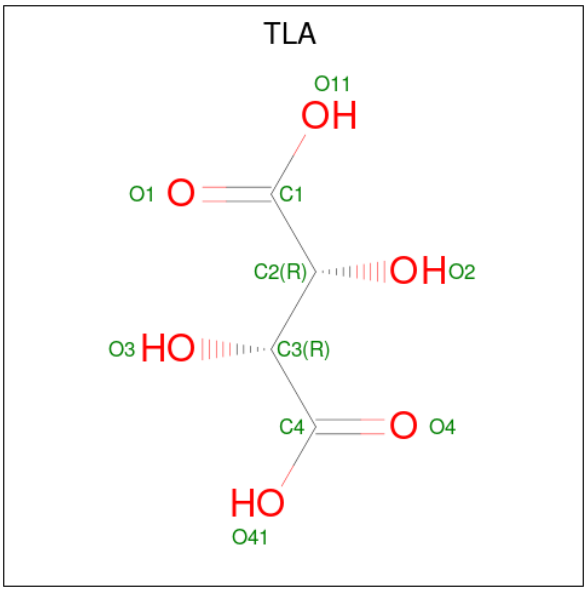
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is 3-DEHYDROSHIKIMATE (three-letter code: DHK) (formula: $C_7H_{10}O_5$).



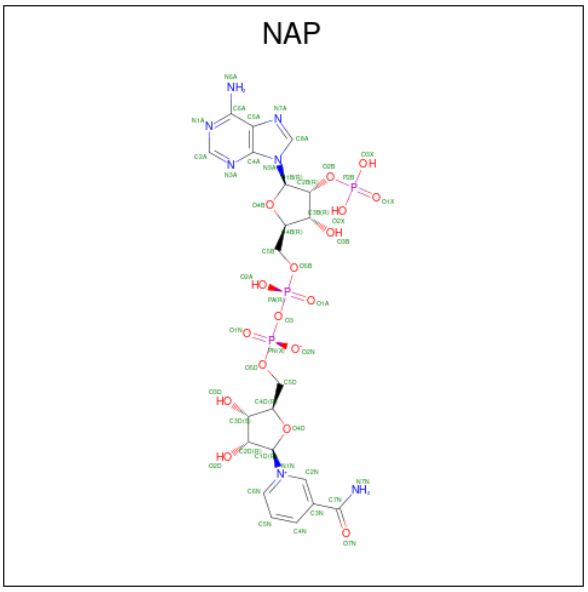
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 7 4	0	1
3	A	1	Total C O 12 7 5	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

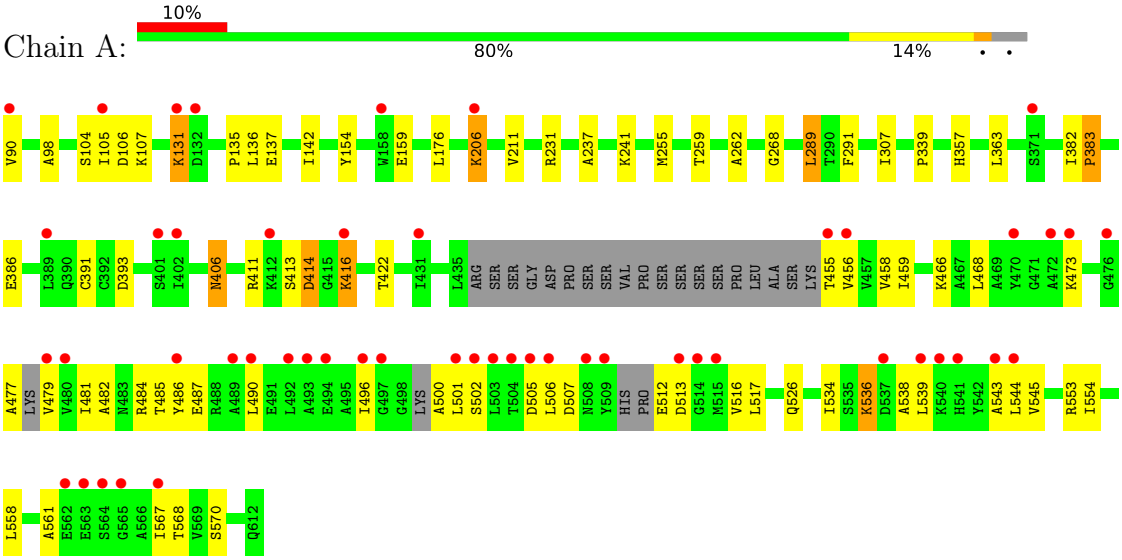
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	205	Total	O	0	0
			205	205		

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: Bifunctional 3-dehydroquinate dehydratase/shikimate dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.45Å 97.45Å 116.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.78 44.95 – 1.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.78) 92.0 (44.95-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.233 0.228 , 0.260	Depositor DCC
R_{free} test set	2894 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4150	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, CSO, NAP, DHK, 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	0.32	0/3910	0.60	1/5282 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	LEU	CA-CB-CG	5.15	127.14	115.30

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	3859	0	3877	73	0
2	A	5	0	0	0	0
3	A	23	0	15	1	0
4	A	10	0	4	1	0
5	A	48	0	25	1	0
6	A	205	0	0	6	0
All	All	4150	0	3921	73	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 9.

All (73) 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:255:MET:HE1	1:A:268:GLY:HA3	1.50	0.93
1:A:545:VAL:HG11	1:A:561:ALA:HB1	1.53	0.90
1:A:411:ARG:NH2	1:A:416:LYS:HD2	1.95	0.82
1:A:105:ILE:HD11	1:A:142:ILE:HG13	1.65	0.79
1:A:411:ARG:HH21	1:A:416:LYS:HD2	1.49	0.77
1:A:545:VAL:HG11	1:A:561:ALA:CB	2.14	0.77
1:A:241[B]:LYS:NZ	4:A:1241[B]:TLA:O1	2.23	0.70
1:A:544:LEU:HD23	1:A:545:VAL:N	2.11	0.65
1:A:255:MET:HE3	1:A:255:MET:O	1.96	0.64
1:A:206:LYS:H	1:A:206:LYS:HD3	1.61	0.64
1:A:416:LYS:NZ	1:A:416:LYS:HB3	2.15	0.62
1:A:414:ASP:OD1	1:A:416:LYS:HG2	2.00	0.61
1:A:455:THR:HG21	1:A:512:GLU:OE2	2.02	0.60
1:A:406:ASN:HD21	1:A:422:THR:H	1.49	0.59
1:A:459:ILE:HD11	1:A:517:LEU:HD11	1.84	0.59
1:A:553:ARG:HD2	6:A:9337:HOH:O	2.02	0.59
1:A:255:MET:CE	1:A:268:GLY:HA3	2.30	0.58
1:A:231:ARG:HD3	6:A:9347:HOH:O	2.03	0.57
1:A:543:ALA:O	1:A:567:ILE:HG22	2.04	0.56
1:A:502:SER:HB3	1:A:505:ASP:OD1	2.07	0.55
1:A:482:ALA:HA	1:A:501:LEU:O	2.06	0.55
1:A:104:SER:OG	1:A:107:LYS:HD3	2.08	0.54
1:A:501:LEU:HD23	1:A:502:SER:N	2.21	0.54
1:A:485:THR:HG22	1:A:487:GLU:HG3	1.89	0.54
1:A:363:LEU:HD12	1:A:391:CSO:SG	2.48	0.54
1:A:131:LYS:HA	1:A:131:LYS:HE3	1.90	0.54
1:A:131:LYS:HE3	1:A:131:LYS:O	2.08	0.53
1:A:255:MET:HE1	1:A:259:THR:HG23	1.90	0.53
1:A:490:LEU:HA	1:A:500:ALA:HB2	1.89	0.53
1:A:484:ARG:HD2	5:A:1411:NAP:O2X	2.09	0.53
1:A:90:VAL:HB	6:A:9282:HOH:O	2.08	0.53
1:A:416:LYS:HB3	1:A:416:LYS:HZ3	1.74	0.53
1:A:291:PHE:CE1	3:A:9241[A]:DHK:H6C1	2.45	0.52
1:A:231:ARG:HG3	6:A:9396:HOH:O	2.11	0.51
1:A:255:MET:CE	1:A:259:THR:HG23	2.41	0.51
1:A:486:TYR:HA	6:A:9378:HOH:O	2.09	0.51
1:A:456:VAL:HA	1:A:516:VAL:HG13	1.93	0.50
1:A:137:GLU:OE1	1:A:137:GLU:N	2.41	0.49
1:A:516:VAL:HG23	1:A:544:LEU:HD22	1.94	0.49
1:A:544:LEU:HD23	1:A:544:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LYS:HD2	1:A:496:ILE:O	2.13	0.49
1:A:526:GLN:NE2	6:A:9414:HOH:O	2.46	0.49
1:A:131:LYS:HE3	1:A:131:LYS:CA	2.43	0.48
1:A:98:ALA:HB2	1:A:307:ILE:HD11	1.95	0.48
1:A:206:LYS:HD3	1:A:206:LYS:N	2.27	0.48
1:A:456:VAL:HG22	1:A:516:VAL:HG11	1.96	0.48
1:A:458:VAL:HB	1:A:481:ILE:HD13	1.96	0.47
1:A:406:ASN:ND2	1:A:422:THR:H	2.12	0.47
1:A:539:LEU:HD13	1:A:561:ALA:HA	1.95	0.47
1:A:544:LEU:HG	1:A:567:ILE:HG23	1.96	0.47
1:A:553:ARG:NH1	1:A:554:ILE:HD11	2.30	0.46
1:A:105:ILE:HG23	1:A:106:ASP:N	2.30	0.46
1:A:473:LYS:HD2	1:A:496:ILE:HB	1.97	0.46
1:A:105:ILE:HD11	1:A:142:ILE:CG1	2.40	0.46
1:A:159:GLU:O	1:A:159:GLU:HG3	2.16	0.46
1:A:363:LEU:C	1:A:363:LEU:HD13	2.36	0.46
1:A:339:PRO:HG2	1:A:357:HIS:CE1	2.51	0.45
1:A:468:LEU:O	1:A:468:LEU:HD23	2.16	0.45
1:A:393:ASP:OD2	1:A:416:LYS:HB2	2.16	0.45
1:A:211:VAL:CG2	1:A:237:ALA:HB2	2.46	0.45
1:A:411:ARG:HH21	1:A:416:LYS:CD	2.25	0.45
1:A:506:LEU:HG	1:A:534:ILE:HD12	1.98	0.45
1:A:386:GLU:OE2	1:A:466:LYS:HE2	2.17	0.44
1:A:558:LEU:HD11	1:A:570:SER:HA	2.00	0.43
1:A:545:VAL:HG13	1:A:568:THR:HG22	2.01	0.43
1:A:477:ALA:O	1:A:479:VAL:HG13	2.19	0.42
1:A:507:ASP:O	1:A:538:ALA:HB2	2.20	0.42
1:A:477:ALA:C	1:A:479:VAL:HG13	2.40	0.41
1:A:406:ASN:HD22	1:A:406:ASN:H	1.68	0.41
1:A:536:LYS:HA	1:A:539:LEU:HG	2.03	0.41
1:A:90:VAL:HG21	1:A:262:ALA:O	2.20	0.41
1:A:255:MET:HE1	1:A:259:THR:CG2	2.51	0.40
1:A:382:ILE:HA	1:A:383:PRO:HA	1.85	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	489/523 (94%)	471 (96%)	16 (3%)	2 (0%)	34 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	SER
1	A	135	PRO

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	417/437 (95%)	405 (97%)	12 (3%)	42 25

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	136	LEU
1	A	154	TYR
1	A	176	LEU
1	A	206	LYS
1	A	289	LEU
1	A	383	PRO
1	A	406	ASN
1	A	414	ASP

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Mol	Chain	Res	Type
1	A	416	LYS
1	A	513	ASP
1	A	536	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	116	HIS
1	A	190	GLN
1	A	234	GLN
1	A	263	GLN
1	A	315	ASN
1	A	368	GLN
1	A	406	ASN
1	A	526	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	CSO	A	391	1	3,6,7	0.57	0	0,6,8	-	-
1	CSO	A	424	1	3,6,7	0.63	0	0,6,8	-	-

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	CSO	A	391	1	-	0/1/5/7	-
1	CSO	A	424	1	-	0/1/5/7	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	391	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
3	DHK	A	4733	-	12,12,12	4.89	7 (58%)	10,17,17	2.06	2 (20%)
3	DHK	A	9241[A]	1	10,11,12	5.67	5 (50%)	9,15,17	3.93	5 (55%)
4	TLA	A	1241[B]	-	9,9,9	0.75	0	12,12,12	1.28	2 (16%)
5	NAP	A	1411	-	45,52,52	2.12	10 (22%)	56,80,80	2.14	13 (23%)
2	SO4	A	1403	-	4,4,4	0.27	0	6,6,6	0.06	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
5	NAP	A	1411	-	1/1/12/12	3/31/67/67	0/5/5/5
3	DHK	A	4733	-	1/1/5/6	1/4/20/20	0/1/1/1
4	TLA	A	1241[B]	-	-	0/12/12/12	-
3	DHK	A	9241[A]	1	3/3/4/6	0/4/17/20	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9241[A]	DHK	C2-C3	14.41	1.55	1.32
3	A	4733	DHK	C2-C3	11.79	1.51	1.32
3	A	4733	DHK	C1-C2	-8.91	1.33	1.50
3	A	9241[A]	DHK	C6-C5	-8.84	1.30	1.52
5	A	1411	NAP	C2N-N1N	5.98	1.42	1.35
5	A	1411	NAP	C2A-N3A	5.82	1.41	1.32
3	A	4733	DHK	C4-C3	5.33	1.56	1.50
5	A	1411	NAP	C5A-C4A	-4.68	1.28	1.40
5	A	1411	NAP	C2A-N1A	4.58	1.42	1.33
3	A	9241[A]	DHK	O1-C	4.21	1.35	1.22
3	A	4733	DHK	O1-C	3.95	1.34	1.22
5	A	1411	NAP	C4A-N3A	3.52	1.40	1.35
5	A	1411	NAP	O4D-C1D	3.41	1.45	1.41
5	A	1411	NAP	C6N-N1N	3.21	1.43	1.35
3	A	4733	DHK	C5-C4	2.94	1.55	1.52
5	A	1411	NAP	C2N-C3N	2.91	1.43	1.39
5	A	1411	NAP	C4N-C3N	2.86	1.44	1.39
3	A	9241[A]	DHK	O2-C	-2.85	1.21	1.30
3	A	9241[A]	DHK	O3-C3	2.43	1.44	1.30
5	A	1411	NAP	P2B-O2X	-2.42	1.45	1.54
3	A	4733	DHK	O3-C3	2.34	1.43	1.30
3	A	4733	DHK	O2-C	-2.21	1.23	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	9241[A]	DHK	C6-C5-C4	8.48	120.18	110.94
5	A	1411	NAP	O3B-C3B-C2B	6.75	130.34	111.17
3	A	9241[A]	DHK	C5-C6-C1	6.39	121.57	111.53
5	A	1411	NAP	C3N-C2N-N1N	-5.92	114.64	120.43
5	A	1411	NAP	N3A-C2A-N1A	-5.49	120.09	128.68
3	A	4733	DHK	C6-C1-C2	4.52	123.22	107.71
5	A	1411	NAP	PN-O3-PA	-4.15	118.59	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4733	DHK	O3-C3-C2	-3.81	108.54	121.96
5	A	1411	NAP	C5B-C4B-C3B	3.76	129.29	115.18
3	A	9241[A]	DHK	O3-C3-C2	-3.45	109.80	121.96
5	A	1411	NAP	C2N-C3N-C4N	3.35	122.06	118.26
5	A	1411	NAP	C4A-C5A-N7A	3.22	112.75	109.40
5	A	1411	NAP	C6N-N1N-C2N	2.93	124.64	121.97
5	A	1411	NAP	C3D-C2D-C1D	2.69	105.03	100.98
5	A	1411	NAP	O5B-PA-O1A	2.56	119.07	109.07
4	A	1241[B]	TLA	O11-C1-C2	2.47	119.95	113.27
5	A	1411	NAP	O7N-C7N-N7N	-2.45	119.09	122.58
5	A	1411	NAP	C1B-N9A-C4A	2.36	130.79	126.64
4	A	1241[B]	TLA	O41-C4-C3	2.31	119.51	113.27
3	A	9241[A]	DHK	C1-C2-C3	-2.15	109.10	119.71
3	A	9241[A]	DHK	O2-C-O1	-2.06	119.42	124.09
5	A	1411	NAP	C3N-C7N-N7N	2.05	120.21	117.75

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	9241[A]	DHK	C4
3	A	9241[A]	DHK	C5
3	A	9241[A]	DHK	C1
3	A	4733	DHK	C1
5	A	1411	NAP	C1B

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1411	NAP	C5B-O5B-PA-O1A
5	A	1411	NAP	O4B-C4B-C5B-O5B
3	A	4733	DHK	O2-C-C1-C2
5	A	1411	NAP	C3B-C4B-C5B-O5B

There are no ring outliers.

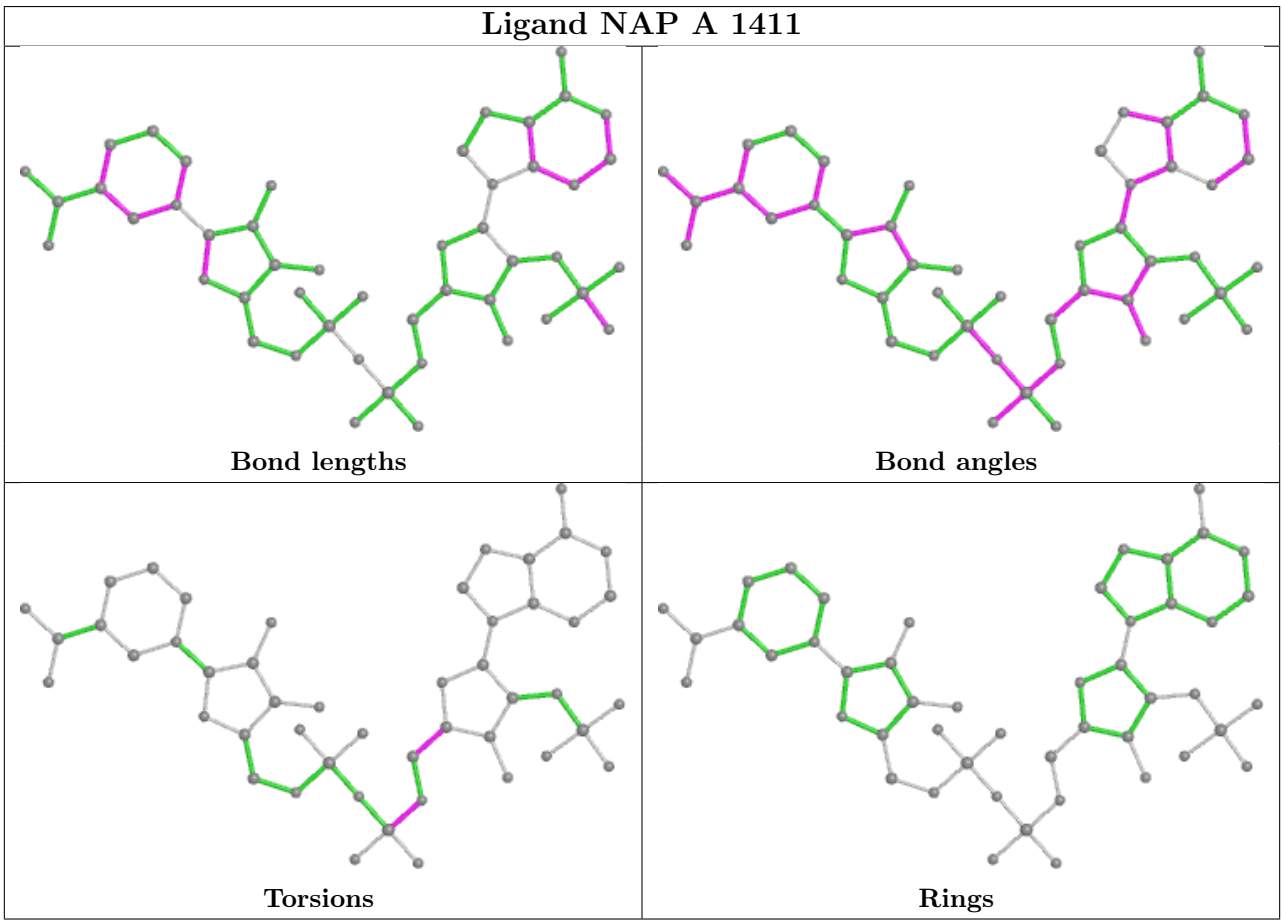
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9241[A]	DHK	1	0
4	A	1241[B]	TLA	1	0
5	A	1411	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAP A 1411



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, 95^{th} 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%)	0.50	51 (10%)	6 6	17, 29, 56, 76	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	LEU	8.5
1	A	90	VAL	7.6
1	A	540	LYS	5.8
1	A	480	VAL	5.7
1	A	496	ILE	5.3
1	A	508	ASN	5.2
1	A	514	GLY	5.1
1	A	489	ALA	4.9
1	A	504	THR	4.7
1	A	455	THR	4.4
1	A	567	ILE	4.0
1	A	502	SER	3.7
1	A	513	ASP	3.7
1	A	206	LYS	3.6
1	A	505	ASP	3.6
1	A	543	ALA	3.3
1	A	541	HIS	3.3
1	A	476	GLY	3.3
1	A	494	GLU	3.2
1	A	503	LEU	3.2
1	A	131	LYS	3.1
1	A	537	ASP	3.1
1	A	501	LEU	3.0
1	A	456	VAL	3.0
1	A	389	LEU	2.9
1	A	562	GLU	2.8
1	A	544	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	401	SER	2.7
1	A	486	TYR	2.7
1	A	539	LEU	2.7
1	A	493	ALA	2.6
1	A	479	VAL	2.6
1	A	473	LYS	2.5
1	A	472	ALA	2.5
1	A	565	GLY	2.5
1	A	515	MET	2.4
1	A	371	SER	2.4
1	A	564	SER	2.4
1	A	416	LYS	2.3
1	A	412	LYS	2.3
1	A	509	TYR	2.2
1	A	402	ILE	2.2
1	A	497	GLY	2.2
1	A	431	ILE	2.1
1	A	470	TYR	2.1
1	A	158	TRP	2.1
1	A	506	LEU	2.1
1	A	563	GLU	2.1
1	A	105	ILE	2.0
1	A	132	ASP	2.0
1	A	492	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
1	CSO	A	391	7/8	0.88	0.10	40,41,44,46	0
1	CSO	A	424	7/8	0.91	0.09	26,28,32,36	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

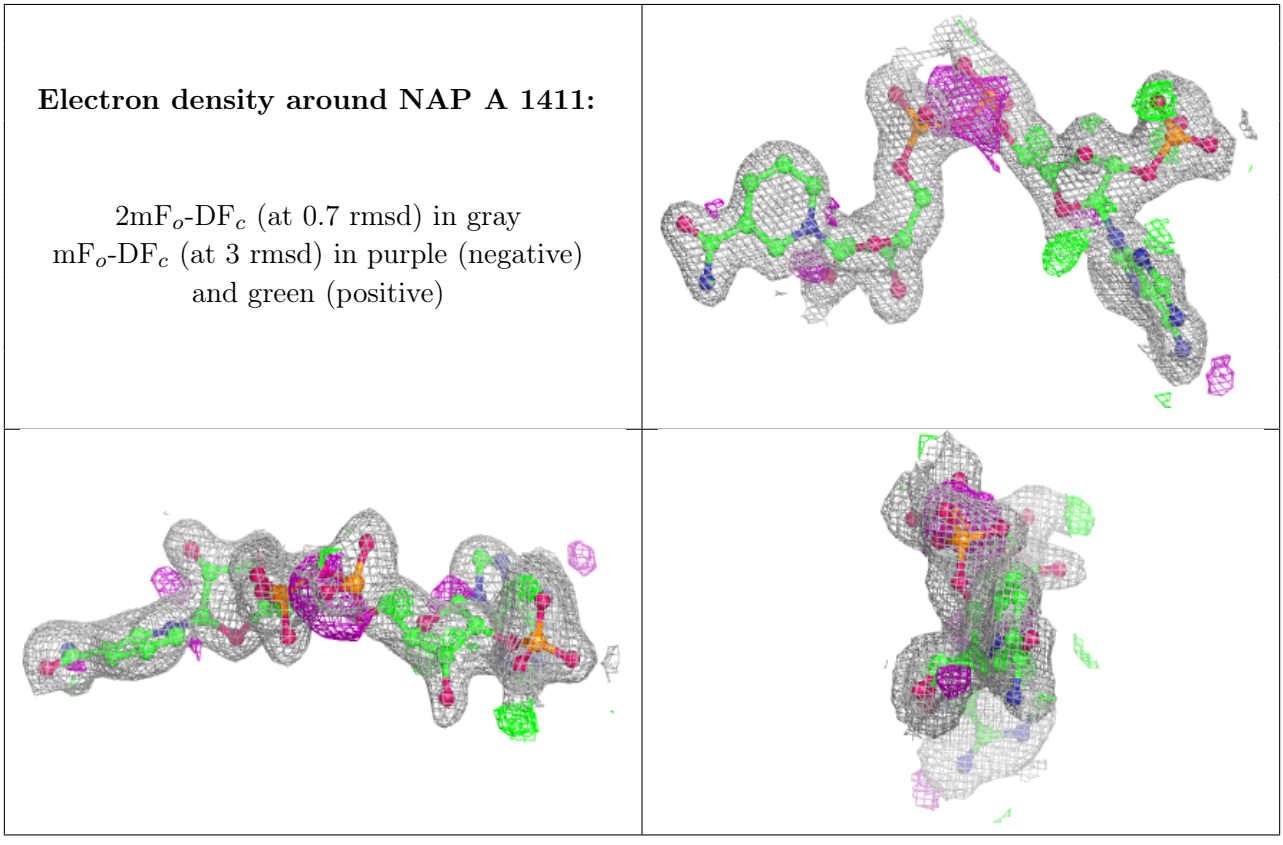
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1403	5/5	0.83	0.31	45,45,49,50	5
5	NAP	A	1411	48/48	0.86	0.13	27,39,52,53	0
3	DHK	A	9241[A]	11/12	0.89	0.16	16,23,25,25	11
4	TLA	A	1241[B]	10/10	0.91	0.16	19,24,27,28	10
3	DHK	A	4733	12/12	0.96	0.09	20,25,30,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP A 1411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.