



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:31 PM GMT

PDB ID : 3ZOK
Title : Structure of 3-Dehydroquinate Synthase from *Actinidia chinensis* in complex with NAD
Authors : Mittelstaedt, G.; Negron, L.; Schofield, L.R.; Marsh, K.; Parker, E.J.
Deposited on : 2013-02-22
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

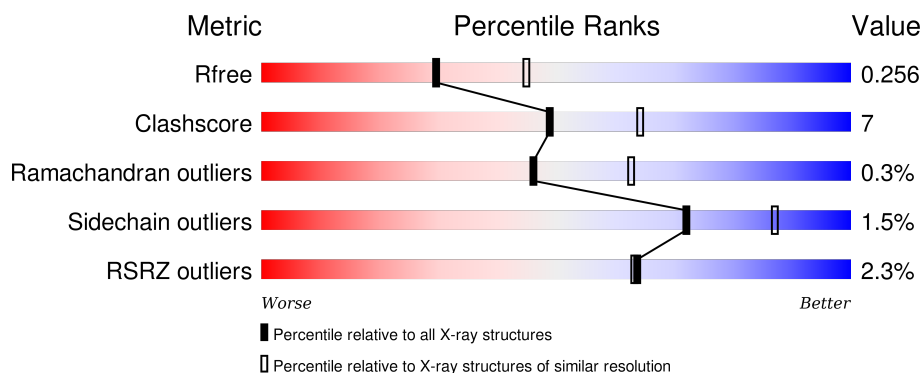
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	378	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	B	378	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	C	378	<div> <div>3%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	D	378	<div> <div>%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

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
2	PO4	A	1380	-	-	-	X
2	PO4	B	1380	-	-	-	X
2	PO4	D	1380	-	-	-	X
4	PEG	D	1383	-	-	-	X
5	GLY	D	1387	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11573 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 SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2760	1752	474	516	18			
1	B	365	Total	C	N	O	S	0	0	0
			2758	1748	470	522	18			
1	C	365	Total	C	N	O	S	0	0	0
			2752	1744	474	516	18			
1	D	365	Total	C	N	O	S	0	0	0
			2768	1755	474	521	18			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



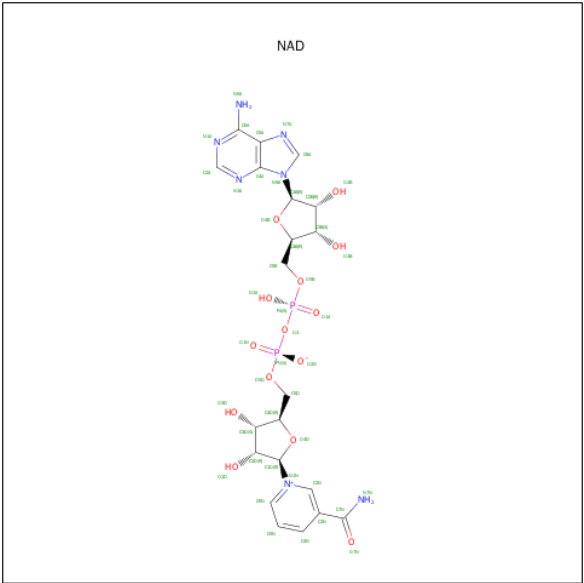
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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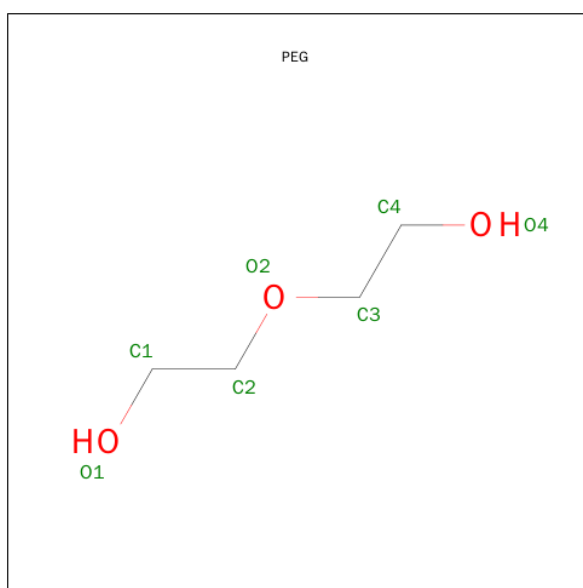
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



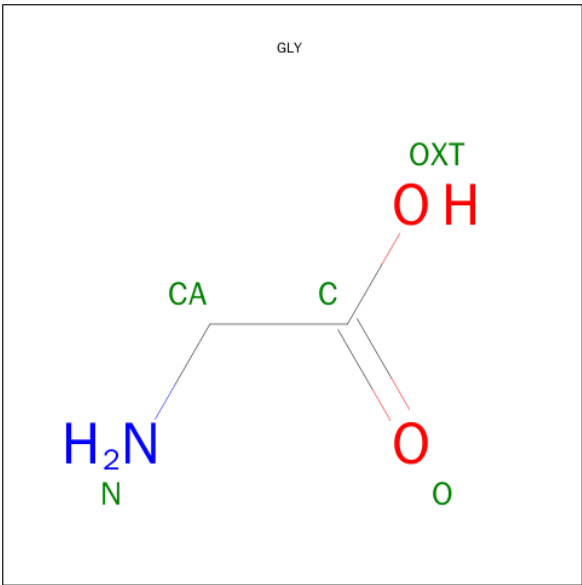
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



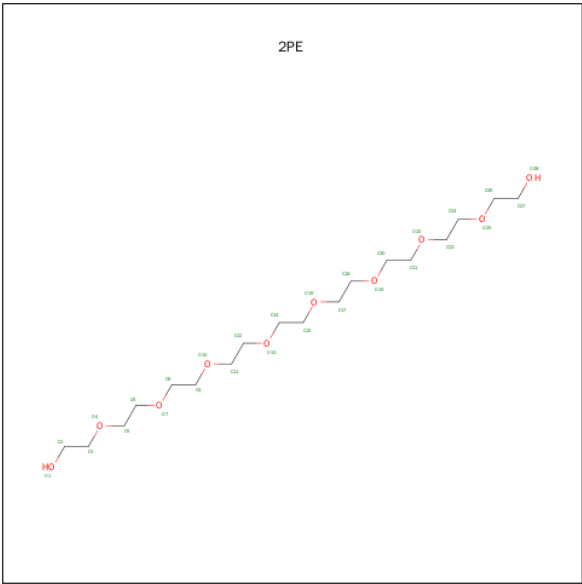
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



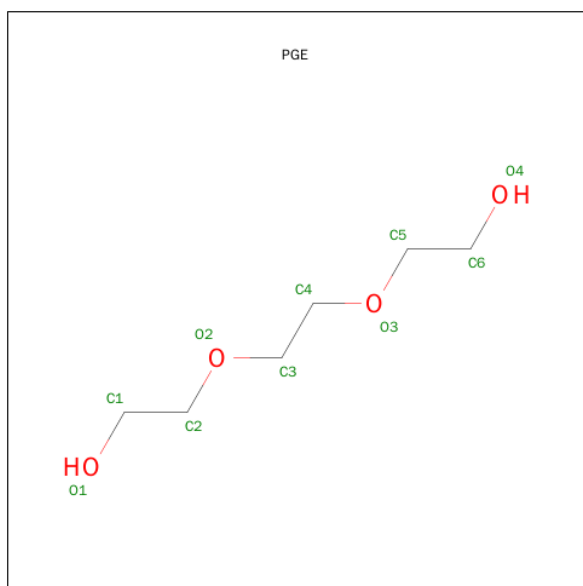
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	2	1	2		
5	B	1	Total	C	N	O	0	0
			5	2	1	2		
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



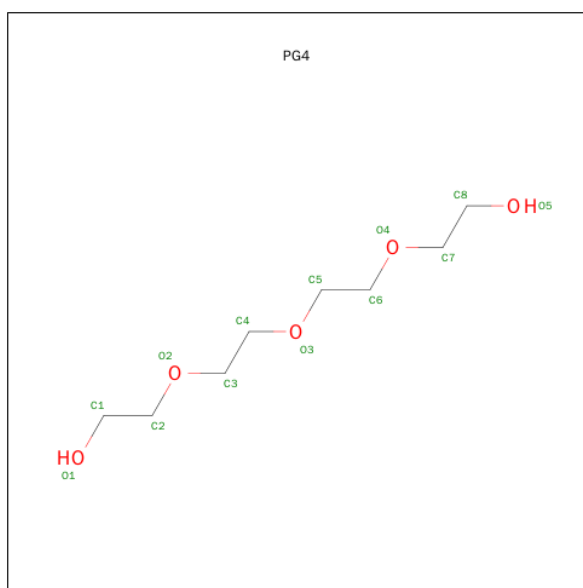
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			25	16	9		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	8	5		

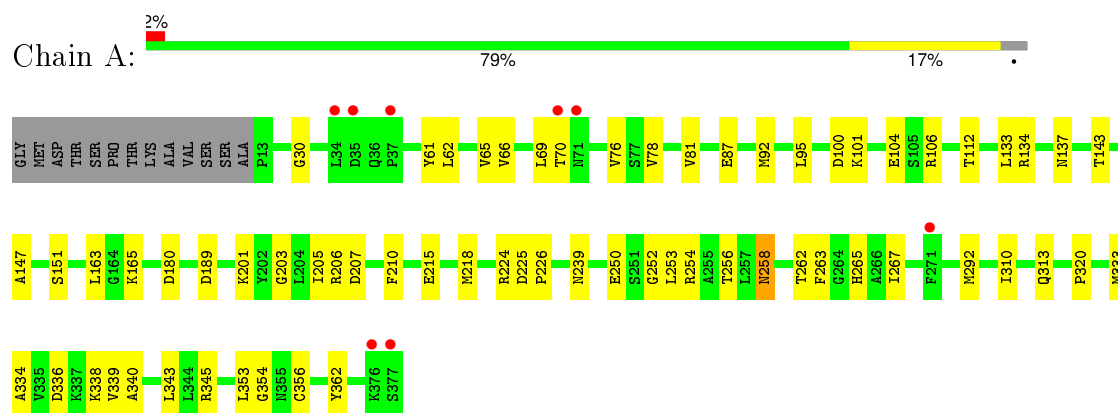
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	48	Total	O	0	0
			48	48		
9	B	40	Total	O	0	0
			40	40		
9	C	53	Total	O	0	0
			53	53		
9	D	40	Total	O	0	0
			40	40		

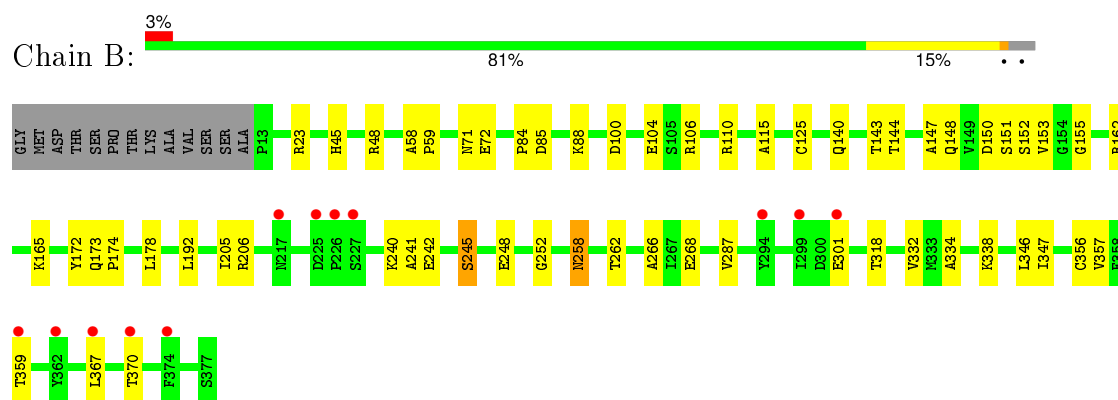
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

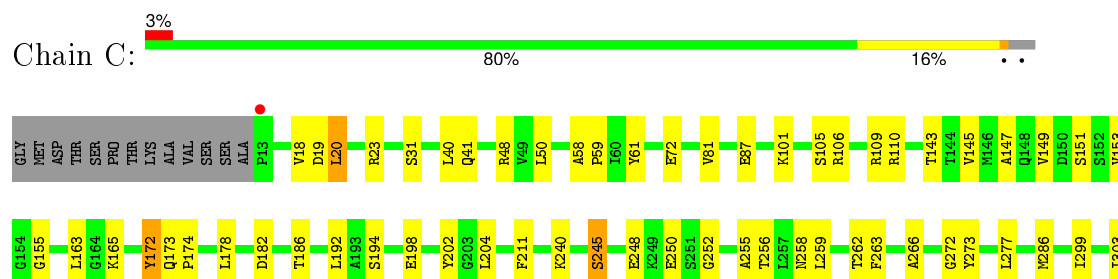
• Molecule 1: 3-DEHYDROQUINATE SYNTHASE

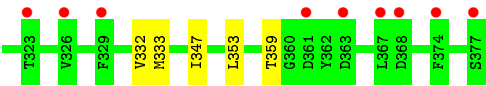


• Molecule 1: 3-DEHYDROQUINATE SYNTHASE

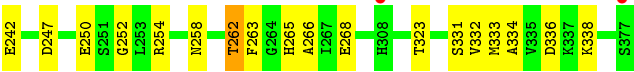
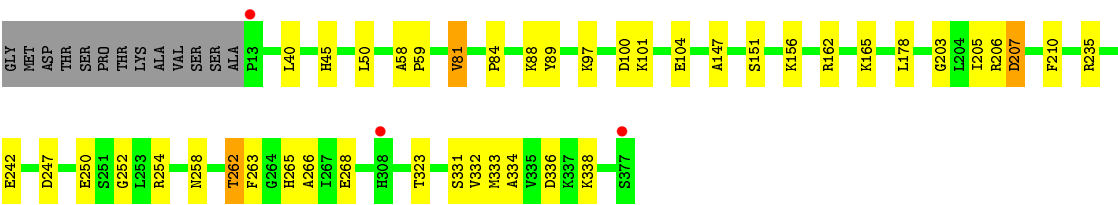
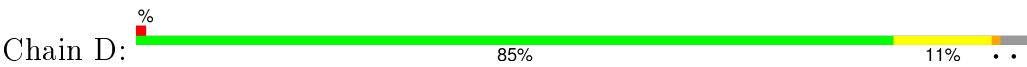


• Molecule 1: 3-DEHYDROQUINATE SYNTHASE





● Molecule 1: 3-DEHYDROQUINATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.06 Å 150.97 Å 84.75 Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	45.50 – 2.40 45.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.50-2.40) 99.5 (45.46-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.253 0.195 , 0.256	Depositor DCC
R_{free} test set	2834 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55593 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11573	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PGE, NAD, PO4, PG4, 2PE, PEG

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	0.52	1/2811 (0.0%)	0.67	1/3814 (0.0%)
1	B	0.52	1/2808 (0.0%)	0.68	3/3812 (0.1%)
1	C	0.54	1/2802 (0.0%)	0.70	2/3802 (0.1%)
1	D	0.56	0/2819	0.69	1/3825 (0.0%)
All	All	0.53	3/11240 (0.0%)	0.69	7/15253 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	PRO	N-CD	5.39	1.55	1.47
1	C	174	PRO	N-CD	5.36	1.55	1.47
1	A	226	PRO	N-CD	5.11	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	GLY	N-CA-C	-5.71	98.83	113.10
1	A	225	ASP	C-N-CD	5.67	140.31	128.40
1	D	81	VAL	CB-CA-C	-5.62	100.73	111.40
1	C	173	GLN	C-N-CD	5.53	140.00	128.40
1	B	173	GLN	C-N-CD	5.49	139.93	128.40
1	B	85	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	48	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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	2760	0	2760	43	0
1	B	2758	0	2743	47	0
1	C	2752	0	2746	40	0
1	D	2768	0	2763	32	0
2	A	15	0	0	1	0
2	B	20	0	0	3	0
2	C	15	0	0	2	0
2	D	20	0	0	1	0
3	A	44	0	26	1	0
3	B	44	0	26	2	0
3	C	44	0	26	1	0
3	D	44	0	26	0	0
4	A	14	0	20	1	0
4	D	21	0	30	2	0
5	A	5	0	2	0	0
5	B	5	0	2	1	0
5	C	5	0	2	0	0
5	D	10	0	4	0	0
6	B	25	0	33	2	0
7	B	10	0	14	2	0
8	C	13	0	18	0	0
9	A	48	0	0	1	0
9	B	40	0	0	2	0
9	C	53	0	0	3	0
9	D	40	0	0	2	0
All	All	11573	0	11241	163	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 7.

All (163) 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:71:ASN:O	1:B:72:GLU:HG2	1.47	1.13
1:B:357:VAL:HG12	1:B:359:THR:HG23	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:NH2	1:B:242:GLU:CD	2.25	0.91
1:B:153:VAL:O	1:B:240:LYS:HE2	1.73	0.88
1:B:71:ASN:O	1:B:72:GLU:CG	2.23	0.87
1:A:147:ALA:HA	1:A:151:SER:OG	1.76	0.85
1:D:205:ILE:HG13	1:D:206:ARG:HG2	1.61	0.83
1:C:81:VAL:HG22	1:C:101:LYS:HG2	1.62	0.79
1:B:258:ASN:ND2	1:B:338:LYS:HE2	1.99	0.79
1:B:206:ARG:HH22	1:B:242:GLU:CD	1.87	0.77
1:C:155:GLY:HA3	1:C:172:TYR:O	1.85	0.75
1:B:357:VAL:HG12	1:B:359:THR:CG2	2.18	0.74
1:C:23:ARG:NH2	1:C:248:GLU:OE1	2.21	0.73
1:A:206:ARG:NH1	1:A:239:ASN:OD1	2.20	0.73
1:B:266:ALA:HA	1:B:332:VAL:HG11	1.71	0.73
1:B:357:VAL:CG1	1:B:359:THR:HG23	2.17	0.73
1:B:45:HIS:O	1:B:110:ARG:NH2	2.24	0.71
1:D:262:THR:OG1	1:D:338:LYS:NZ	2.23	0.70
1:C:163:LEU:HD22	4:D:1384:PEG:H22	1.73	0.70
1:A:262:THR:OG1	1:A:338:LYS:NZ	2.21	0.70
1:C:155:GLY:CA	1:C:172:TYR:O	2.40	0.69
1:B:258:ASN:HD22	1:B:338:LYS:HE2	1.58	0.69
1:B:258:ASN:HD22	1:B:338:LYS:CE	2.05	0.69
1:B:262:THR:OG1	1:B:338:LYS:NZ	2.25	0.69
1:C:147:ALA:HA	1:C:151:SER:OG	1.94	0.68
5:B:1385:GLY:N	9:B:2021:HOH:O	2.25	0.68
1:C:143:THR:HB	3:C:1381:NAD:H61A	1.58	0.68
1:C:87:GLU:HG3	1:C:273:TYR:HB3	1.76	0.67
1:D:147:ALA:HA	1:D:151:SER:OG	1.96	0.66
1:D:336:ASP:OD1	1:D:338:LYS:HE3	1.97	0.65
1:A:81:VAL:HG22	1:A:101:LYS:HG2	1.79	0.65
1:D:250:GLU:HG3	1:D:254:ARG:HB3	1.78	0.64
1:B:338:LYS:HD3	1:B:347:ILE:HD11	1.81	0.63
1:D:100:ASP:O	1:D:104:GLU:HG2	1.98	0.63
1:B:357:VAL:CG1	1:B:359:THR:CG2	2.77	0.62
1:D:206:ARG:HH22	1:D:242:GLU:CD	2.02	0.62
1:C:87:GLU:OE2	1:C:165:LYS:NZ	2.31	0.62
1:B:206:ARG:NH2	1:B:242:GLU:OE1	2.26	0.62
1:C:194:SER:OG	1:C:277:LEU:HD12	2.00	0.62
1:B:150:ASP:O	1:B:240:LYS:NZ	2.32	0.61
1:D:81:VAL:HG22	1:D:101:LYS:HG2	1.82	0.60
1:B:150:ASP:OD1	1:B:240:LYS:NZ	2.23	0.59
1:B:153:VAL:O	1:B:240:LYS:CE	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:NH2	1:C:105:SER:O	2.37	0.58
1:C:61:TYR:HH	1:C:186:THR:HG1	1.52	0.58
1:D:263:PHE:CD1	1:D:333:MET:CE	2.86	0.57
1:B:71:ASN:C	1:B:72:GLU:HG2	2.21	0.57
1:A:92:MET:HE1	1:A:95:LEU:HD23	1.86	0.57
1:C:40:LEU:HD21	1:C:178:LEU:HD22	1.86	0.56
1:A:267:ILE:HD11	1:A:320:PRO:HB3	1.88	0.56
1:C:18:VAL:HG12	1:C:20:LEU:HD22	1.87	0.56
1:C:50:LEU:HD11	1:C:81:VAL:HG23	1.86	0.56
1:A:258:ASN:HD22	1:A:338:LYS:HE2	1.71	0.55
1:D:45:HIS:HE1	9:D:2003:HOH:O	1.89	0.55
1:B:338:LYS:HD3	1:B:347:ILE:CD1	2.37	0.55
1:A:265:HIS:HB3	9:A:2029:HOH:O	2.06	0.54
2:C:1378:PO4:O3	2:C:1379:PO4:O3	2.26	0.54
1:B:241:ALA:O	1:B:245:SER:OG	2.24	0.54
1:C:255:ALA:HB1	1:C:347:ILE:HD11	1.89	0.54
1:A:334:ALA:HB1	1:B:106:ARG:HD3	1.89	0.54
1:C:145:VAL:HG21	1:C:192:LEU:HD12	1.88	0.53
1:B:165:LYS:HE2	1:B:268:GLU:OE2	2.08	0.53
1:A:205:ILE:HG13	1:A:206:ARG:N	2.24	0.53
1:D:165:LYS:HG2	1:D:265:HIS:CD2	2.44	0.53
1:A:92:MET:HE3	1:A:95:LEU:HB3	1.90	0.53
1:D:40:LEU:HD21	1:D:178:LEU:HD22	1.90	0.52
2:B:1378:PO4:O2	2:B:1379:PO4:O2	2.28	0.52
1:A:263:PHE:CE1	1:A:333:MET:HE1	2.44	0.52
1:B:258:ASN:ND2	1:B:338:LYS:CE	2.68	0.51
1:B:205:ILE:HG13	1:B:206:ARG:HG2	1.91	0.51
1:C:266:ALA:HA	1:C:332:VAL:HG11	1.90	0.51
1:A:336:ASP:OD1	1:A:338:LYS:HE3	2.11	0.51
1:A:92:MET:CE	1:A:95:LEU:HD23	2.41	0.51
1:A:207:ASP:CG	1:A:210:PHE:HB2	2.30	0.51
1:C:41:GLN:OE1	1:C:72:GLU:OE1	2.29	0.51
1:C:259:LEU:HD23	1:C:286:MET:HE3	1.93	0.50
1:A:61:TYR:O	1:A:65:VAL:HG23	2.10	0.50
1:C:145:VAL:O	1:C:149:VAL:HG22	2.11	0.50
1:D:165:LYS:HE2	1:D:268:GLU:OE1	2.12	0.50
1:C:204:LEU:HD12	1:C:286:MET:CE	2.42	0.50
1:A:87:GLU:OE2	1:A:165:LYS:NZ	2.39	0.50
1:A:253:LEU:O	1:A:256:THR:OG1	2.20	0.50
1:B:84:PRO:HB3	6:B:1383:2PE:C9	2.41	0.50
1:C:110:ARG:HD2	9:C:2003:HOH:O	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HB2	9:B:2007:HOH:O	2.12	0.49
1:A:262:THR:HG22	1:A:333:MET:HG2	1.93	0.49
1:C:18:VAL:HG12	1:C:20:LEU:CD2	2.43	0.49
1:A:203:GLY:HA2	1:A:207:ASP:O	2.12	0.49
1:B:100:ASP:O	1:B:104:GLU:HG2	2.12	0.48
1:A:62:LEU:O	1:A:66:VAL:HG12	2.13	0.48
1:A:70:THR:HG22	1:A:76:VAL:HG12	1.95	0.48
1:C:263:PHE:CE1	1:C:333:MET:HE1	2.48	0.48
1:A:106:ARG:HE	7:B:1384:PGE:H62	1.79	0.48
1:C:256:THR:HA	1:C:347:ILE:HG12	1.96	0.48
1:B:205:ILE:HG13	1:B:206:ARG:N	2.29	0.48
1:A:215:GLU:HA	1:A:310:ILE:HD13	1.95	0.48
1:A:100:ASP:O	1:A:104:GLU:HG2	2.13	0.48
1:A:133:LEU:O	1:A:134:ARG:HB2	2.14	0.47
1:B:258:ASN:HD22	1:B:338:LYS:NZ	2.13	0.47
1:A:201:LYS:O	1:A:205:ILE:HG12	2.15	0.47
2:B:1381:PO4:O2	1:D:97:LYS:NZ	2.33	0.47
1:C:40:LEU:CD2	1:C:178:LEU:HD22	2.45	0.47
1:D:58:ALA:HB3	1:D:59:PRO:HD3	1.96	0.46
1:D:207:ASP:HB3	1:D:210:PHE:HB3	1.96	0.46
1:A:250:GLU:HG3	1:A:254:ARG:HB3	1.98	0.46
1:B:266:ALA:HA	1:B:332:VAL:CG1	2.44	0.46
1:C:198:GLU:O	1:C:202:TYR:CD2	2.68	0.46
1:C:262:THR:HG22	1:C:333:MET:HG2	1.98	0.46
1:B:287:VAL:HG21	1:B:318:THR:HG22	1.98	0.46
1:C:299:ILE:HG13	1:C:303:ILE:HD12	1.98	0.45
1:A:189:ASP:OD1	1:A:224:ARG:NH1	2.49	0.45
2:A:1378:PO4:O2	2:A:1379:PO4:O4	2.34	0.45
1:A:339:VAL:HA	1:A:343:LEU:O	2.16	0.45
1:D:247:ASP:OD2	1:D:250:GLU:HA	2.17	0.45
1:D:266:ALA:HA	1:D:332:VAL:HG11	1.98	0.45
1:C:263:PHE:CE2	2:C:1380:PO4:O3	2.70	0.45
1:D:165:LYS:HE3	1:D:268:GLU:OE2	2.17	0.44
1:B:155:GLY:CA	1:B:172:TYR:O	2.66	0.44
1:D:205:ILE:HG13	1:D:206:ARG:N	2.33	0.44
1:B:58:ALA:HB3	1:B:59:PRO:HD3	1.99	0.44
1:D:88:LYS:HD3	1:D:89:TYR:CZ	2.53	0.44
1:B:162:ARG:CD	1:D:162:ARG:HD2	2.48	0.44
1:B:115:ALA:HB2	1:B:125:CYS:SG	2.58	0.44
1:A:256:THR:HG22	1:A:356:CYS:SG	2.58	0.44
1:B:140:GLN:HG2	1:B:152:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LEU:HD11	1:D:81:VAL:HG23	2.00	0.43
1:D:263:PHE:CD1	1:D:333:MET:HE1	2.53	0.43
1:A:340:ALA:HB2	1:A:345:ARG:CZ	2.49	0.43
1:A:30:GLY:O	1:A:180:ASP:HA	2.18	0.43
1:D:235:ARG:HD3	2:D:1381:PO4:O2	2.18	0.43
1:D:50:LEU:HD11	1:D:81:VAL:CG2	2.49	0.43
1:D:323:THR:O	1:D:323:THR:CG2	2.66	0.43
1:C:353:LEU:HD12	9:C:2042:HOH:O	2.18	0.43
1:C:106:ARG:NH2	9:C:2012:HOH:O	2.51	0.43
1:B:147:ALA:HA	1:B:151:SER:OG	2.19	0.43
1:A:206:ARG:HA	1:A:354:GLY:O	2.19	0.42
1:C:109:ARG:HH12	1:D:250:GLU:HB3	1.85	0.42
1:B:144:THR:O	1:B:148:GLN:HG3	2.18	0.42
1:A:163:LEU:HB3	4:A:1383:PEG:H32	2.01	0.42
1:B:143:THR:HB	3:B:1382:NAD:H61A	1.84	0.42
1:A:143:THR:HB	3:A:1381:NAD:H61A	1.83	0.42
1:D:203:GLY:HA2	1:D:207:ASP:HB3	2.02	0.42
1:C:19:ASP:O	1:C:245:SER:HB3	2.19	0.42
1:A:218:MET:HG2	1:A:313:GLN:HB3	2.00	0.42
1:C:31:SER:OG	1:C:182:ASP:OD1	2.28	0.42
1:D:156:LYS:HB2	9:D:2028:HOH:O	2.20	0.42
1:A:112:THR:HA	1:A:137:ASN:O	2.19	0.41
1:B:23:ARG:NH2	1:B:248:GLU:OE1	2.37	0.41
1:C:153:VAL:O	1:C:240:LYS:HE2	2.20	0.41
1:D:334:ALA:HA	4:D:1385:PEG:H32	2.02	0.41
1:B:346:LEU:HD22	2:B:1380:PO4:O4	2.21	0.41
1:A:205:ILE:HG13	1:A:206:ARG:HG2	2.03	0.41
1:B:334:ALA:HA	7:B:1384:PGE:H22	2.03	0.41
1:B:151:SER:HA	3:B:1382:NAD:C4N	2.51	0.41
1:C:58:ALA:HB3	1:C:59:PRO:HD3	2.02	0.41
1:A:258:ASN:ND2	1:A:338:LYS:HE2	2.35	0.41
1:A:65:VAL:O	1:A:69:LEU:HD13	2.21	0.41
1:C:250:GLU:HG2	1:C:250:GLU:O	2.20	0.41
1:B:367:LEU:O	1:B:370:THR:HG22	2.21	0.41
6:B:1383:2PE:H151	1:D:84:PRO:HG3	2.03	0.40
1:A:70:THR:CG2	1:A:78:VAL:HG23	2.51	0.40
1:A:292:MET:HE1	1:A:362:TYR:CD1	2.56	0.40
1:C:211:PHE:CD2	1:C:353:LEU:HD21	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	363/378 (96%)	352 (97%)	10 (3%)	1 (0%)	46	63
1	B	363/378 (96%)	355 (98%)	7 (2%)	1 (0%)	46	63
1	C	363/378 (96%)	350 (96%)	12 (3%)	1 (0%)	46	63
1	D	363/378 (96%)	353 (97%)	9 (2%)	1 (0%)	46	63
All	All	1452/1512 (96%)	1410 (97%)	38 (3%)	4 (0%)	46	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLY
1	B	252	GLY
1	C	252	GLY
1	D	252	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	293/312 (94%)	291 (99%)	2 (1%)	88	95
1	B	293/312 (94%)	287 (98%)	6 (2%)	63	81
1	C	291/312 (93%)	286 (98%)	5 (2%)	68	85
1	D	295/312 (95%)	291 (99%)	4 (1%)	74	88
All	All	1172/1248 (94%)	1155 (98%)	17 (2%)	72	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	353	LEU
1	B	178	LEU
1	B	192	LEU
1	B	245	SER
1	B	258	ASN
1	B	301	GLU
1	B	356	CYS
1	C	20	LEU
1	C	172	TYR
1	C	245	SER
1	C	258	ASN
1	C	359	THR
1	D	207	ASP
1	D	258	ASN
1	D	262	THR
1	D	331	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	372	HIS
1	B	217	ASN
1	B	258	ASN
1	C	258	ASN
1	D	45	HIS
1	D	209	ASN
1	D	258	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

31 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	PO4	A	1378	-	4,4,4	0.88	0	6,6,6	0.31	0
2	PO4	A	1379	-	4,4,4	0.52	0	6,6,6	0.25	0
2	PO4	A	1380	-	4,4,4	0.27	0	6,6,6	0.32	0
3	NAD	A	1381	-	38,48,48	0.88	1 (2%)	47,73,73	1.61	5 (10%)
4	PEG	A	1382	-	6,6,6	0.58	0	5,5,5	0.38	0
4	PEG	A	1383	-	6,6,6	0.57	0	5,5,5	0.63	0
5	GLY	A	1384	-	1,4,4	0.89	0	0,4,4	0.00	-
2	PO4	B	1378	-	4,4,4	0.60	0	6,6,6	0.30	0
2	PO4	B	1379	-	4,4,4	0.60	0	6,6,6	0.27	0
2	PO4	B	1380	-	4,4,4	0.56	0	6,6,6	0.28	0
2	PO4	B	1381	-	4,4,4	0.57	0	6,6,6	0.27	0
3	NAD	B	1382	-	38,48,48	0.86	1 (2%)	47,73,73	1.53	4 (8%)
6	2PE	B	1383	-	24,24,27	0.49	0	23,23,26	0.51	0
7	PGE	B	1384	-	9,9,9	0.69	0	8,8,8	0.40	0
5	GLY	B	1385	-	1,4,4	0.79	0	0,4,4	0.00	-
2	PO4	C	1378	-	4,4,4	0.41	0	6,6,6	0.28	0
2	PO4	C	1379	-	4,4,4	0.60	0	6,6,6	0.27	0
2	PO4	C	1380	-	4,4,4	0.35	0	6,6,6	0.28	0
3	NAD	C	1381	-	38,48,48	0.81	1 (2%)	47,73,73	1.60	4 (8%)
8	PG4	C	1382	-	12,12,12	0.60	0	11,11,11	0.30	0
5	GLY	C	1383	-	1,4,4	0.92	0	0,4,4	0.00	-
2	PO4	D	1378	-	4,4,4	0.67	0	6,6,6	0.31	0
2	PO4	D	1379	-	4,4,4	0.63	0	6,6,6	0.29	0
2	PO4	D	1380	-	4,4,4	0.44	0	6,6,6	0.28	0
2	PO4	D	1381	-	4,4,4	0.56	0	6,6,6	0.28	0
3	NAD	D	1382	-	38,48,48	0.96	2 (5%)	47,73,73	1.39	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	D	1383	-	6,6,6	0.50	0	5,5,5	0.14	0
4	PEG	D	1384	-	6,6,6	0.62	0	5,5,5	0.61	0
4	PEG	D	1385	-	6,6,6	0.44	0	5,5,5	0.42	0
5	GLY	D	1386	-	1,4,4	0.89	0	0,4,4	0.00	-
5	GLY	D	1387	-	1,4,4	0.87	0	0,4,4	0.00	-

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	PO4	A	1378	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1379	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1380	-	-	0/0/0/0	0/0/0/0
3	NAD	A	1381	-	-	0/22/62/62	0/5/5/5
4	PEG	A	1382	-	-	0/4/4/4	0/0/0/0
4	PEG	A	1383	-	-	0/4/4/4	0/0/0/0
5	GLY	A	1384	-	-	0/0/2/2	0/0/0/0
2	PO4	B	1378	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1379	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1380	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1381	-	-	0/0/0/0	0/0/0/0
3	NAD	B	1382	-	-	0/22/62/62	0/5/5/5
6	2PE	B	1383	-	-	0/22/22/25	0/0/0/0
7	PGE	B	1384	-	-	0/7/7/7	0/0/0/0
5	GLY	B	1385	-	-	0/0/2/2	0/0/0/0
2	PO4	C	1378	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1379	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1380	-	-	0/0/0/0	0/0/0/0
3	NAD	C	1381	-	-	0/22/62/62	0/5/5/5
8	PG4	C	1382	-	-	0/10/10/10	0/0/0/0
5	GLY	C	1383	-	-	0/0/2/2	0/0/0/0
2	PO4	D	1378	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1379	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1380	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1381	-	-	0/0/0/0	0/0/0/0
3	NAD	D	1382	-	-	0/22/62/62	0/5/5/5
4	PEG	D	1383	-	-	0/4/4/4	0/0/0/0
4	PEG	D	1384	-	-	0/4/4/4	0/0/0/0
4	PEG	D	1385	-	-	0/4/4/4	0/0/0/0
5	GLY	D	1386	-	-	0/0/2/2	0/0/0/0
5	GLY	D	1387	-	-	0/0/2/2	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1382	NAD	O7N-C7N	-2.14	1.19	1.24
3	C	1381	NAD	C5A-C4A	2.21	1.45	1.40
3	A	1381	NAD	C5A-C4A	2.39	1.45	1.40
3	B	1382	NAD	C5A-C4A	2.43	1.46	1.40
3	D	1382	NAD	C5A-C4A	2.48	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1381	NAD	N3A-C2A-N1A	-7.73	122.97	128.89
3	C	1381	NAD	N3A-C2A-N1A	-7.34	123.27	128.89
3	B	1382	NAD	N3A-C2A-N1A	-6.97	123.56	128.89
3	D	1382	NAD	N3A-C2A-N1A	-6.56	123.87	128.89
3	B	1382	NAD	C4A-C5A-N7A	-3.44	106.31	109.48
3	C	1381	NAD	C4A-C5A-N7A	-3.16	106.57	109.48
3	A	1381	NAD	O3-PN-O5D	-3.16	94.56	102.94
3	A	1381	NAD	C4A-C5A-N7A	-3.11	106.62	109.48
3	D	1382	NAD	C4A-C5A-N7A	-2.96	106.76	109.48
3	B	1382	NAD	C1B-N9A-C4A	-2.42	123.30	126.94
3	C	1381	NAD	C1B-N9A-C4A	-2.20	123.62	126.94
3	D	1382	NAD	O7N-C7N-N7N	-2.02	119.75	122.59
3	A	1381	NAD	C2A-N1A-C6A	2.06	122.45	118.77
3	A	1381	NAD	O2N-PN-O3	2.19	115.01	105.09
3	D	1382	NAD	C3N-C7N-N7N	2.56	120.61	117.82
3	B	1382	NAD	O4D-C1D-N1N	2.93	111.35	108.13
3	C	1381	NAD	O4D-C1D-N1N	3.53	112.01	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1378	PO4	1	0
2	A	1379	PO4	1	0
3	A	1381	NAD	1	0
4	A	1383	PEG	1	0
2	B	1378	PO4	1	0
2	B	1379	PO4	1	0
2	B	1380	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1381	PO4	1	0
3	B	1382	NAD	2	0
6	B	1383	2PE	2	0
7	B	1384	PGE	2	0
5	B	1385	GLY	1	0
2	C	1378	PO4	1	0
2	C	1379	PO4	1	0
2	C	1380	PO4	1	0
3	C	1381	NAD	1	0
2	D	1381	PO4	1	0
4	D	1384	PEG	1	0
4	D	1385	PEG	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	365/378 (96%)	0.03	8 (2%) 65 64	20, 31, 48, 68	0
1	B	365/378 (96%)	0.27	12 (3%) 50 50	19, 34, 52, 64	0
1	C	365/378 (96%)	0.14	10 (2%) 58 57	19, 36, 56, 84	0
1	D	365/378 (96%)	-0.07	3 (0%) 87 87	18, 28, 41, 53	0
All	All	1460/1512 (96%)	0.09	33 (2%) 64 63	18, 32, 51, 84	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	SER	4.1
1	A	35	ASP	3.5
1	B	359	THR	3.2
1	D	377	SER	3.2
1	A	34	LEU	2.7
1	B	294	TYR	2.7
1	B	226	PRO	2.6
1	B	370	THR	2.5
1	C	368	ASP	2.5
1	C	377	SER	2.5
1	B	225	ASP	2.5
1	B	374	PHE	2.4
1	D	13	PRO	2.4
1	C	363	ASP	2.4
1	B	362	TYR	2.4
1	A	376	LYS	2.4
1	A	71	ASN	2.3
1	C	367	LEU	2.2
1	C	323	THR	2.2
1	C	13	PRO	2.2
1	B	217	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	301	GLU	2.2
1	B	299	ILE	2.1
1	A	271	PHE	2.1
1	A	70	THR	2.1
1	C	361	ASP	2.1
1	B	367	LEU	2.1
1	C	374	PHE	2.1
1	A	37	PRO	2.1
1	A	377	SER	2.1
1	C	326	VAL	2.0
1	D	308	HIS	2.0
1	C	329	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	D	1380	5/5	0.96	0.26	5.41	40,40,46,50	0
2	PO4	B	1380	5/5	0.94	0.35	5.33	60,61,65,69	0
2	PO4	A	1380	5/5	0.94	0.23	4.32	32,33,39,42	0
5	GLY	D	1387	5/5	0.84	0.23	3.46	47,49,52,55	0
4	PEG	D	1383	7/7	0.83	0.23	2.83	40,43,45,46	0
6	2PE	B	1383	25/28	0.93	0.22	1.73	31,34,41,43	0
8	PG4	C	1382	13/13	0.88	0.26	1.59	35,42,46,47	0
5	GLY	A	1384	5/5	0.97	0.17	1.57	19,20,21,21	0
2	PO4	A	1378	5/5	0.98	0.16	0.65	27,30,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	C	1380	5/5	0.98	0.19	0.63	37,37,45,46	0
7	PGE	B	1384	10/10	0.92	0.20	0.61	37,40,41,42	0
5	GLY	B	1385	5/5	0.97	0.15	0.17	25,27,31,35	0
5	GLY	C	1383	5/5	0.97	0.14	0.08	26,29,31,33	0
4	PEG	A	1383	7/7	0.87	0.18	0.07	37,38,42,42	0
4	PEG	D	1384	7/7	0.86	0.18	0.07	40,41,42,43	0
4	PEG	D	1385	7/7	0.93	0.15	-0.13	37,38,44,47	0
3	NAD	A	1381	44/44	0.94	0.14	-0.14	19,28,34,34	0
3	NAD	D	1382	44/44	0.96	0.13	-0.28	17,21,23,24	0
3	NAD	B	1382	44/44	0.95	0.14	-0.33	21,24,28,30	0
4	PEG	A	1382	7/7	0.95	0.15	-0.78	39,40,42,42	0
5	GLY	D	1386	5/5	0.89	0.13	-0.79	45,45,46,48	0
3	NAD	C	1381	44/44	0.96	0.12	-0.81	20,27,34,38	0
2	PO4	D	1378	5/5	0.99	0.11	-0.88	27,28,30,31	0
2	PO4	A	1379	5/5	0.99	0.11	-0.99	28,28,32,33	0
2	PO4	D	1379	5/5	0.99	0.11	-1.17	25,26,28,28	0
2	PO4	B	1379	5/5	0.99	0.11	-1.20	32,32,35,35	0
2	PO4	B	1378	5/5	0.99	0.12	-1.21	28,28,30,31	0
2	PO4	C	1378	5/5	0.99	0.10	-2.12	32,33,36,39	0
2	PO4	C	1379	5/5	0.99	0.10	-2.31	24,24,25,26	0
2	PO4	B	1381	5/5	0.92	0.18	-	56,59,62,66	0
2	PO4	D	1381	5/5	0.91	0.24	-	64,68,70,72	0

6.5 Other polymers

There are no such residues in this entry.