



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:28 PM UTC

PDB ID : 4QUV / pdb_00004quv
Title : Structure of an integral membrane delta(14)-sterol reductase
Authors : Li, X.; Blobel, G.
Deposited on : 2014-07-12
Resolution : 2.74 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

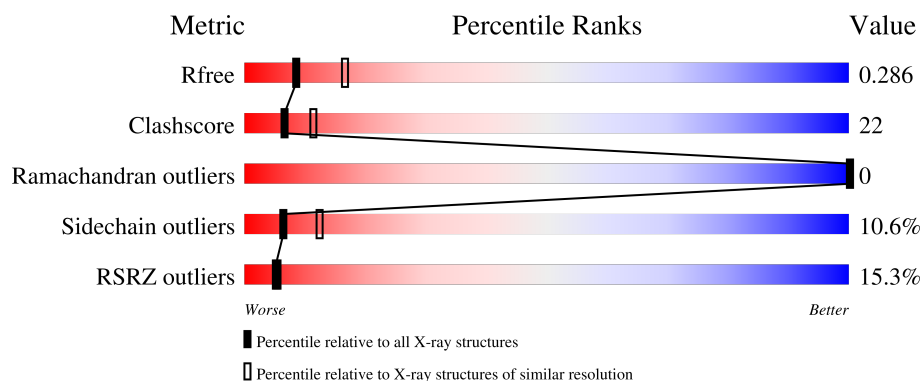
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	427	16% 57% 30% 5% 8%
1	B	427	12% 54% 33% • 9%

2 Entry composition [i](#)

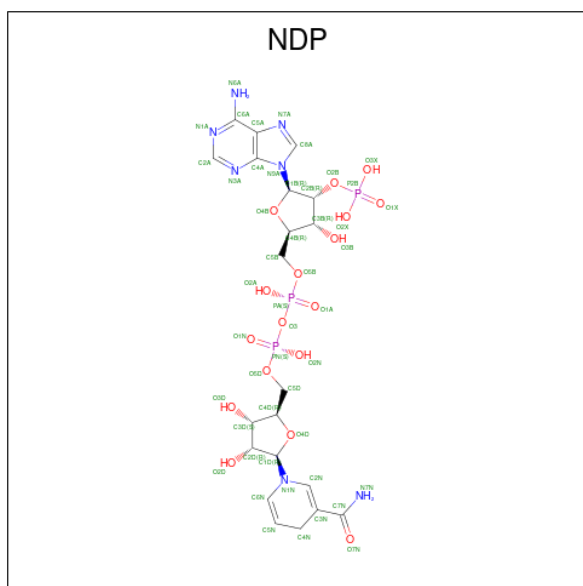
There are 2 unique types of molecules in this entry. The entry contains 6490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3235	2181	520	516	18			
1	B	389	Total	C	N	O	S	0	0	0
			3193	2149	515	511	18			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

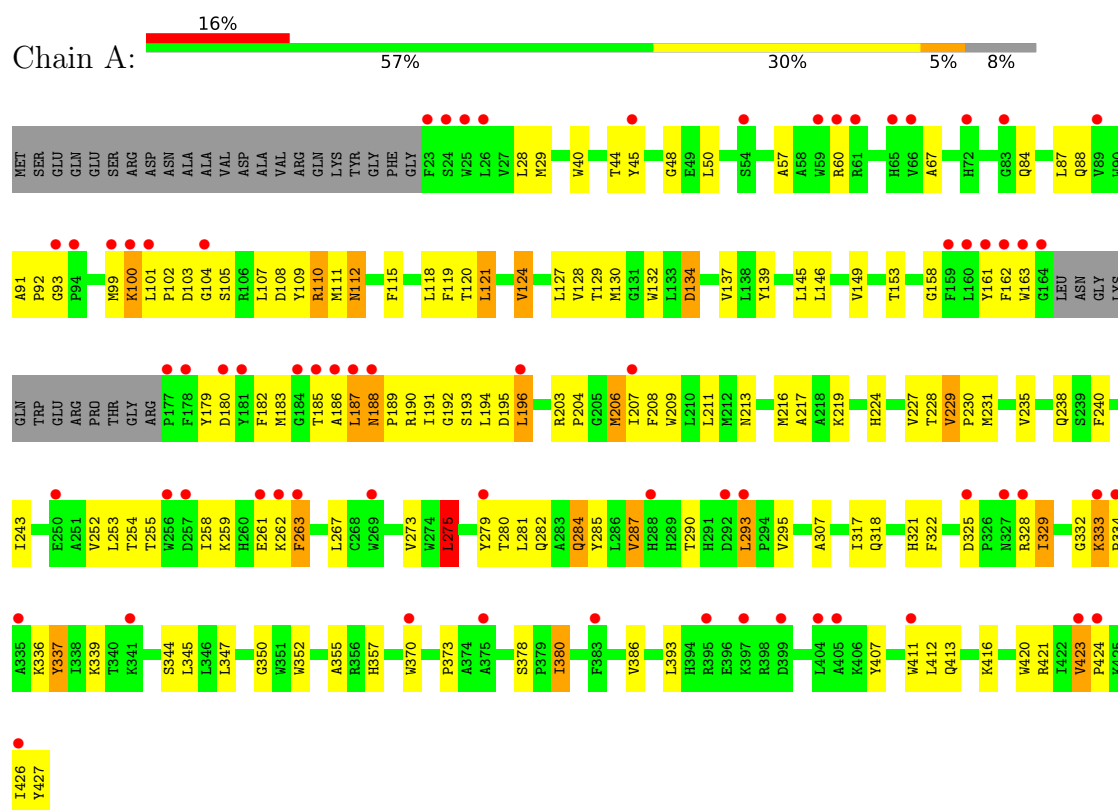


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

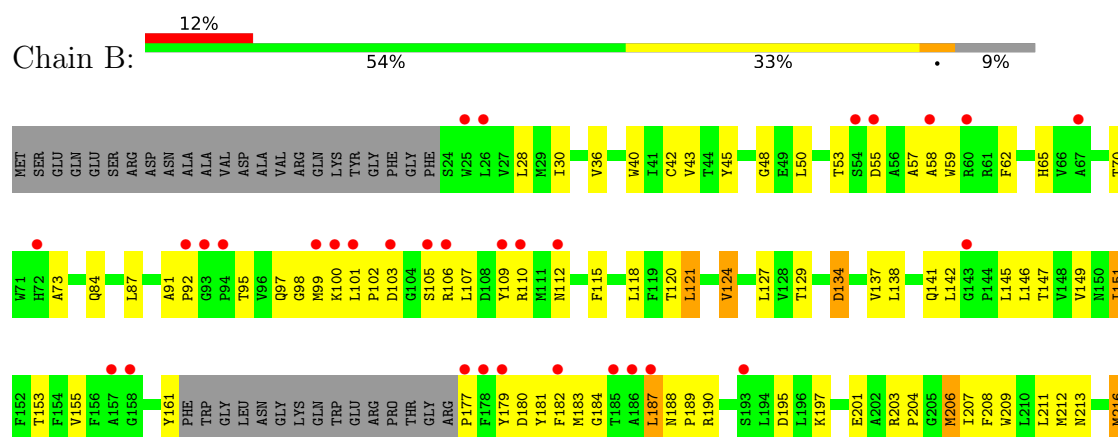
3 Residue-property plots

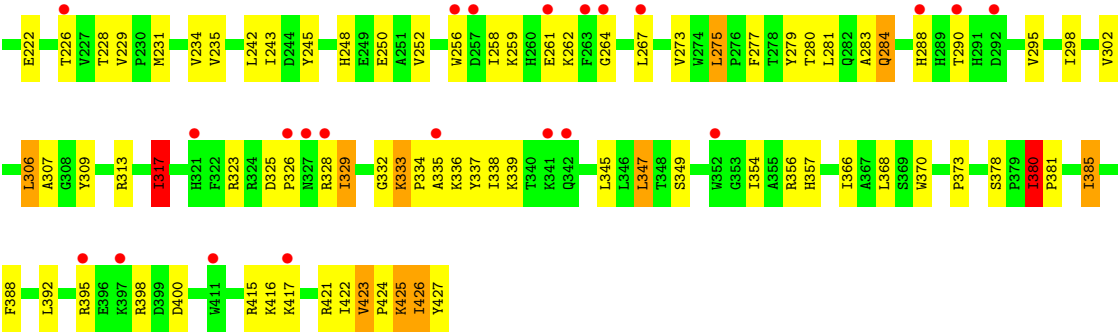
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Delta(14)-sterol reductase



- Molecule 1: Delta(14)-sterol reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.66Å 74.61Å 79.55Å 66.00° 90.37° 86.86°	Depositor
Resolution (Å)	37.26 – 2.74 37.26 – 2.74	Depositor EDS
% Data completeness (in resolution range)	74.5 (37.26-2.74) 74.5 (37.26-2.74)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.233 , 0.284 0.244 , 0.286	Depositor DCC
R_{free} test set	1527 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.5	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	0.89	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: NDP

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	0.59	0/3360	1.04	18/4590 (0.4%)
1	B	0.64	0/3314	1.08	14/4527 (0.3%)
All	All	0.62	0/6674	1.06	32/9117 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	ILE	N-CA-C	8.25	119.24	111.48
1	A	423	VAL	N-CA-C	8.11	122.08	112.35
1	B	325	ASP	N-CA-C	6.73	114.28	108.22
1	B	380	ILE	CB-CA-C	-6.60	107.43	113.70
1	A	101	LEU	CA-C-N	-6.54	113.93	120.21
1	A	101	LEU	C-N-CA	-6.54	113.93	120.21
1	B	426	ILE	CB-CA-C	-6.33	106.33	111.71
1	A	188	ASN	CA-C-N	6.02	125.93	119.85
1	A	188	ASN	C-N-CA	6.02	125.93	119.85
1	B	307	ALA	N-CA-C	-5.85	104.98	111.36
1	B	326	PRO	N-CA-C	-5.80	104.38	113.78
1	A	67	ALA	CA-C-N	5.70	126.25	120.38
1	A	67	ALA	C-N-CA	5.70	126.25	120.38
1	B	329	ILE	N-CA-C	5.67	115.71	108.12
1	B	275	LEU	CA-C-N	-5.67	112.76	119.84
1	B	275	LEU	C-N-CA	-5.67	112.76	119.84
1	A	128	VAL	N-CA-C	5.64	115.84	110.42
1	A	273	VAL	N-CA-C	5.64	116.78	111.48
1	B	332	GLY	N-CA-C	5.58	119.43	112.73
1	B	423	VAL	CA-C-N	-5.44	113.31	118.97
1	B	423	VAL	C-N-CA	-5.44	113.31	118.97
1	A	275	LEU	CA-C-N	-5.42	113.06	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	LEU	C-N-CA	-5.42	113.06	119.84
1	A	273	VAL	CB-CA-C	-5.38	107.14	111.71
1	A	229	VAL	CA-C-N	-5.27	113.10	118.85
1	A	229	VAL	C-N-CA	-5.27	113.10	118.85
1	A	380	ILE	CB-CA-C	-5.26	108.70	113.70
1	A	386	VAL	N-CA-C	-5.26	105.20	110.30
1	B	273	VAL	N-CA-C	5.26	116.42	111.48
1	A	111	MET	N-CA-C	5.08	117.25	107.44
1	B	317	ILE	N-CA-CB	5.07	117.44	110.54
1	A	307	ALA	N-CA-C	-5.04	105.87	111.36

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	3235	0	3203	160	0
1	B	3193	0	3168	122	0
2	A	31	0	11	2	0
2	B	31	0	11	1	0
All	All	6490	0	6393	278	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 22.

All (278) 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:158:GLY:O	1:A:162:PHE:CD2	1.93	1.21
1:A:190:ARG:NH1	1:A:195:ASP:HB2	1.54	1.21
1:A:190:ARG:CZ	1:A:195:ASP:HB2	1.73	1.17
1:A:107:LEU:HD21	1:A:190:ARG:NH2	1.61	1.15
1:A:107:LEU:HD11	1:A:190:ARG:HE	1.13	1.03
1:A:107:LEU:CD2	1:A:190:ARG:NH2	2.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LYS:CG	1:B:334:PRO:HD2	1.97	0.94
1:A:333:LYS:HE2	1:A:336:LYS:HZ1	1.32	0.94
1:B:99:MET:HE2	1:B:259:LYS:HD3	1.50	0.93
1:A:103:ASP:HB3	1:A:105:SER:CB	1.99	0.93
1:A:104:GLY:N	1:A:105:SER:HB3	1.85	0.92
1:A:118:LEU:HD13	1:B:121:LEU:HB3	1.52	0.91
1:A:187:LEU:O	1:A:189:PRO:HD3	1.69	0.91
1:A:158:GLY:O	1:A:162:PHE:HD2	1.41	0.91
1:A:420:TRP:CB	1:A:424:PRO:HB2	1.99	0.90
1:B:188:ASN:OD1	1:B:197:LYS:CD	2.20	0.90
1:A:107:LEU:CD2	1:A:190:ARG:HH21	1.86	0.88
1:A:333:LYS:CE	1:A:336:LYS:HZ1	1.87	0.88
1:A:91:ALA:HB1	1:A:112:ASN:HB3	1.56	0.88
1:A:420:TRP:CD2	1:A:424:PRO:O	2.28	0.86
1:A:57:ALA:HA	1:A:60:ARG:HD3	1.58	0.85
1:A:206:MET:HG3	1:A:275:LEU:HD21	1.59	0.84
1:A:190:ARG:NH1	1:A:195:ASP:CB	2.41	0.83
1:A:333:LYS:HE2	1:A:336:LYS:NZ	1.92	0.82
1:A:107:LEU:HD11	1:A:190:ARG:NE	1.95	0.82
1:B:333:LYS:CD	1:B:334:PRO:HD2	2.10	0.81
1:B:187:LEU:O	1:B:189:PRO:HD3	1.79	0.81
1:A:192:GLY:O	1:A:193:SER:OG	1.99	0.80
1:B:188:ASN:OD1	1:B:197:LYS:HD3	1.79	0.80
1:A:99:MET:HE2	1:A:259:LYS:CD	2.11	0.80
1:B:328:ARG:O	1:B:335:ALA:N	2.14	0.80
1:A:355:ALA:HB2	1:A:424:PRO:HB3	1.62	0.79
1:A:99:MET:HE2	1:A:259:LYS:HD3	1.65	0.78
1:B:99:MET:HG3	1:B:259:LYS:HD3	1.65	0.78
1:B:92:PRO:O	1:B:112:ASN:ND2	2.16	0.78
1:B:188:ASN:OD1	1:B:197:LYS:HD2	1.81	0.78
1:B:99:MET:HE2	1:B:259:LYS:CD	2.13	0.77
1:A:420:TRP:HB2	1:A:424:PRO:HB2	1.64	0.77
1:A:107:LEU:HD22	1:A:109:TYR:CZ	2.21	0.76
1:A:103:ASP:HB3	1:A:105:SER:HB3	1.66	0.75
1:A:333:LYS:HG2	1:A:334:PRO:HD2	1.67	0.75
1:A:321:HIS:NE2	1:B:226:THR:HG22	2.00	0.75
1:A:103:ASP:OD2	1:A:105:SER:HB2	1.87	0.74
1:B:333:LYS:HD3	1:B:334:PRO:HD2	1.68	0.74
1:A:84:GLN:HE21	1:A:203:ARG:HB3	1.53	0.73
1:A:423:VAL:HG23	1:A:427:TYR:C	2.12	0.73
1:A:91:ALA:O	1:A:110:ARG:CZ	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TRP:CB	1:A:424:PRO:CB	2.67	0.72
1:A:107:LEU:HD21	1:A:190:ARG:CZ	2.20	0.71
1:A:107:LEU:HD22	1:A:109:TYR:CE2	2.25	0.71
1:A:190:ARG:NH2	1:A:195:ASP:HB2	2.04	0.71
1:A:355:ALA:HB2	1:A:424:PRO:CB	2.19	0.71
1:A:337:TYR:HD1	1:A:337:TYR:H	1.39	0.70
1:B:55:ASP:O	1:B:57:ALA:N	2.20	0.70
1:A:355:ALA:HB2	1:A:424:PRO:HG3	1.73	0.70
1:A:333:LYS:CD	1:A:336:LYS:NZ	2.55	0.70
1:A:190:ARG:HH12	1:A:195:ASP:HB2	1.52	0.69
1:B:28:LEU:HD23	1:B:182:PHE:HZ	1.57	0.69
1:A:329:ILE:HG22	1:A:332:GLY:O	1.93	0.69
1:A:337:TYR:CD2	1:A:345:LEU:HD22	2.28	0.69
1:B:231:MET:HE1	1:B:283:ALA:HA	1.74	0.68
1:A:103:ASP:HB3	1:A:105:SER:HB2	1.75	0.68
1:B:333:LYS:HG2	1:B:334:PRO:HD2	1.75	0.68
1:A:158:GLY:C	1:A:162:PHE:CD2	2.71	0.68
1:A:99:MET:HG3	1:A:259:LYS:HG2	1.76	0.67
1:B:180:ASP:O	1:B:184:GLY:N	2.28	0.67
1:A:355:ALA:CB	1:A:424:PRO:HB3	2.25	0.67
1:B:99:MET:CE	1:B:259:LYS:HD3	2.24	0.66
1:B:336:LYS:HB2	1:B:349:SER:HB3	1.77	0.66
1:B:333:LYS:CB	1:B:334:PRO:HD2	2.26	0.66
1:A:91:ALA:HB1	1:A:112:ASN:CB	2.25	0.66
1:A:149:VAL:O	1:A:153:THR:HG23	1.96	0.65
1:A:333:LYS:CD	1:A:336:LYS:HZ1	2.09	0.65
1:A:355:ALA:HB2	1:A:424:PRO:CG	2.26	0.65
1:A:158:GLY:C	1:A:162:PHE:HD2	2.04	0.65
1:B:187:LEU:HD22	1:B:262:LYS:HG2	1.80	0.65
1:A:420:TRP:HB3	1:A:424:PRO:CB	2.27	0.64
1:A:206:MET:O	1:A:209:TRP:HB3	1.98	0.64
1:B:99:MET:HG3	1:B:259:LYS:CD	2.28	0.64
1:A:420:TRP:CG	1:A:424:PRO:O	2.50	0.63
1:A:423:VAL:HG11	1:A:426:ILE:HB	1.80	0.63
1:B:213:ASN:HB3	1:B:235:VAL:HG22	1.80	0.63
1:B:231:MET:HA	1:B:231:MET:HE3	1.81	0.62
1:A:158:GLY:O	1:A:162:PHE:CE2	2.50	0.62
1:B:231:MET:HE2	1:B:235:VAL:HG23	1.82	0.62
1:A:216:MET:SD	1:A:284:GLN:HG3	2.40	0.62
1:B:183:MET:HA	1:B:264:GLY:HA3	1.80	0.62
1:B:101:LEU:N	1:B:102:PRO:HD2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD23	1:A:108:ASP:O	2.00	0.61
1:A:420:TRP:CE3	1:A:424:PRO:O	2.54	0.61
1:B:252:VAL:O	1:B:258:ILE:HG13	2.00	0.61
1:A:91:ALA:O	1:A:110:ARG:NE	2.33	0.61
1:A:99:MET:HE2	1:A:259:LYS:HD2	1.83	0.61
1:A:104:GLY:H	1:A:105:SER:HB3	1.64	0.60
1:B:425:LYS:HB3	1:B:426:ILE:HD12	1.84	0.60
1:B:58:ALA:O	1:B:62:PHE:N	2.32	0.60
1:A:121:LEU:HB3	1:B:118:LEU:HD13	1.84	0.59
1:A:107:LEU:HD22	1:A:190:ARG:HH21	1.66	0.58
1:A:216:MET:HE1	1:A:280:THR:HB	1.83	0.58
1:B:395:ARG:HG3	1:B:398:ARG:HH22	1.67	0.58
1:B:112:ASN:OD1	1:B:115:PHE:HB3	2.03	0.58
1:B:206:MET:HG3	1:B:275:LEU:HD21	1.85	0.58
1:B:149:VAL:O	1:B:153:THR:HG23	2.04	0.58
1:A:139:TYR:HD2	1:A:216:MET:HG2	1.70	0.57
1:A:420:TRP:CG	1:A:424:PRO:HB2	2.40	0.57
1:B:161:TYR:HE1	1:B:180:ASP:HB2	1.68	0.57
1:A:161:TYR:HE1	1:A:180:ASP:HB2	1.68	0.57
1:A:337:TYR:CD1	1:A:337:TYR:N	2.72	0.57
1:A:93:GLY:N	1:A:112:ASN:OD1	2.28	0.57
1:B:216:MET:SD	1:B:284:GLN:HG3	2.45	0.56
1:A:107:LEU:HD22	1:A:190:ARG:NH2	2.17	0.56
1:A:423:VAL:CG2	1:A:427:TYR:H	2.19	0.56
1:B:97:GLN:HB3	1:B:106:ARG:HG2	1.86	0.56
1:A:134:ASP:O	1:A:137:VAL:HG23	2.06	0.56
1:B:147:THR:O	1:B:151:ILE:HG23	2.06	0.56
1:B:124:VAL:HG11	1:B:211:LEU:HD22	1.88	0.56
1:A:185:THR:O	1:A:186:ALA:HB3	2.06	0.56
1:A:420:TRP:HB2	1:A:424:PRO:CB	2.31	0.55
1:A:183:MET:O	1:A:262:LYS:O	2.24	0.55
1:B:357:HIS:N	1:B:421:ARG:O	2.39	0.55
1:A:333:LYS:HD3	1:A:336:LYS:NZ	2.22	0.55
1:B:101:LEU:N	1:B:102:PRO:CD	2.68	0.55
1:A:99:MET:CE	1:A:259:LYS:HD3	2.35	0.55
1:B:378:SER:O	1:B:381:PRO:HD2	2.07	0.55
1:B:102:PRO:O	1:B:103:ASP:HB3	2.07	0.54
1:A:190:ARG:CZ	1:A:195:ASP:CB	2.67	0.54
1:B:43:VAL:HA	1:B:48:GLY:HA2	1.88	0.54
1:A:333:LYS:CE	1:A:336:LYS:NZ	2.58	0.54
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD13	1:B:277:PHE:CD2	2.43	0.53
1:A:329:ILE:CG2	1:A:332:GLY:O	2.56	0.53
1:B:187:LEU:O	1:B:189:PRO:CD	2.56	0.53
1:B:338:ILE:HD11	1:B:417:LYS:HG3	1.89	0.53
1:B:177:PRO:HB2	1:B:179:TYR:HD1	1.74	0.52
1:A:139:TYR:CE2	1:A:287:VAL:HG11	2.44	0.52
1:A:228:THR:HG21	1:A:290:THR:HA	1.90	0.52
1:B:134:ASP:O	1:B:137:VAL:HG23	2.09	0.52
1:B:228:THR:HG21	1:B:290:THR:HA	1.92	0.52
1:A:99:MET:HE3	1:A:100:LYS:H	1.74	0.52
1:B:99:MET:HG3	1:B:259:LYS:HG2	1.92	0.52
1:A:48:GLY:O	1:A:378:SER:OG	2.22	0.52
1:A:407:TYR:HB2	1:A:411:TRP:HB2	1.92	0.52
1:A:107:LEU:CD2	1:A:108:ASP:O	2.59	0.51
1:A:252:VAL:O	1:A:255:THR:HG22	2.11	0.51
1:B:84:GLN:HB3	1:B:203:ARG:HB3	1.93	0.51
1:A:325:ASP:HB3	1:A:328:ARG:HG3	1.93	0.51
1:A:28:LEU:HD23	1:A:182:PHE:HZ	1.76	0.51
1:A:413:GLN:HA	1:A:416:LYS:HD2	1.92	0.51
1:A:423:VAL:HG21	1:A:427:TYR:N	2.26	0.50
1:A:370:TRP:O	1:A:373:PRO:HD2	2.11	0.50
1:B:40:TRP:CE3	1:B:142:LEU:HD22	2.47	0.50
1:B:115:PHE:CD1	1:B:115:PHE:C	2.88	0.50
1:A:285:TYR:CE2	1:A:378:SER:HB3	2.46	0.50
1:A:88:GLN:HA	1:A:203:ARG:HH12	1.77	0.50
1:A:179:TYR:O	1:A:182:PHE:N	2.38	0.50
1:B:347:LEU:HD22	1:B:349:SER:H	1.76	0.50
1:A:100:LYS:HB3	1:A:105:SER:OG	2.12	0.50
1:B:101:LEU:HD22	1:B:106:ARG:HH22	1.76	0.50
1:A:321:HIS:CE1	1:B:226:THR:HG22	2.48	0.49
1:A:84:GLN:HB3	1:A:203:ARG:HB3	1.93	0.49
1:A:275:LEU:HD12	1:A:279:TYR:CZ	2.47	0.49
1:B:36:VAL:HG12	1:B:146:LEU:HD21	1.94	0.49
1:A:254:THR:O	1:A:259:LYS:HE2	2.12	0.49
1:A:318:GLN:OE1	1:A:350:GLY:HA3	2.12	0.49
1:B:99:MET:HG3	1:B:259:LYS:CG	2.42	0.49
1:B:309:TYR:HA	1:B:366:ILE:HD11	1.94	0.49
1:B:368:LEU:HD13	1:B:385:ILE:HG13	1.94	0.49
1:B:91:ALA:HB1	1:B:112:ASN:HB3	1.94	0.48
1:A:99:MET:HG2	1:A:253:LEU:O	2.14	0.48
1:A:115:PHE:CD1	1:A:115:PHE:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:HG21	1:A:427:TYR:H	1.79	0.48
2:A:501:NDP:H8A	2:A:501:NDP:H3B	1.96	0.48
1:B:40:TRP:CZ3	1:B:142:LEU:HD22	2.49	0.48
1:A:103:ASP:CB	1:A:105:SER:HB2	2.42	0.48
1:B:161:TYR:CE1	1:B:180:ASP:HB2	2.48	0.48
1:A:217:ALA:HA	1:A:231:MET:HE3	1.95	0.48
1:B:385:ILE:HD13	1:B:385:ILE:HA	1.59	0.47
1:B:107:LEU:HD22	1:B:190:ARG:NH2	2.29	0.47
1:B:298:ILE:O	1:B:302:VAL:HG22	2.15	0.47
1:A:213:ASN:HB3	1:A:235:VAL:HG23	1.96	0.47
1:B:275:LEU:O	1:B:279:TYR:HB2	2.14	0.47
1:B:356:ARG:NH1	1:B:415:ARG:HG2	2.30	0.47
1:B:400:ASP:OD1	1:B:415:ARG:NH2	2.48	0.47
1:B:231:MET:HE1	1:B:283:ALA:CA	2.44	0.47
1:B:101:LEU:HB2	1:B:102:PRO:HD3	1.97	0.47
1:A:99:MET:HG3	1:A:259:LYS:CG	2.43	0.47
1:A:322:PHE:CG	1:A:347:LEU:HD13	2.50	0.47
1:B:87:LEU:O	1:B:91:ALA:N	2.47	0.46
1:A:224:HIS:CG	1:A:290:THR:HG21	2.50	0.46
1:A:413:GLN:O	1:A:416:LYS:HB2	2.15	0.46
1:B:190:ARG:HG2	1:B:195:ASP:HA	1.98	0.46
1:B:206:MET:O	1:B:209:TRP:HB3	2.15	0.46
1:A:347:LEU:N	2:A:501:NDP:N1A	2.60	0.46
1:B:121:LEU:HD13	1:B:121:LEU:HA	1.69	0.46
1:B:333:LYS:HG2	1:B:334:PRO:CD	2.44	0.46
1:B:354:ILE:HG22	1:B:424:PRO:HG3	1.98	0.46
1:A:231:MET:O	1:A:235:VAL:HG12	2.16	0.46
1:A:99:MET:SD	1:A:259:LYS:HD3	2.55	0.46
1:B:100:LYS:HD2	1:B:105:SER:O	2.14	0.46
1:B:138:LEU:HB3	1:B:212:MET:HG2	1.96	0.46
1:A:40:TRP:O	1:A:44:THR:OG1	2.31	0.46
1:B:99:MET:HB3	1:B:100:LYS:H	1.62	0.45
1:B:313:ARG:O	1:B:317:ILE:HG23	2.17	0.45
1:B:99:MET:CG	1:B:259:LYS:HD3	2.40	0.45
1:B:388:PHE:CE2	1:B:392:LEU:HD11	2.51	0.45
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.82	0.45
1:A:412:LEU:O	1:A:416:LYS:HG3	2.15	0.45
1:B:302:VAL:O	1:B:306:LEU:HG	2.17	0.45
1:B:333:LYS:CB	1:B:334:PRO:CD	2.93	0.45
1:A:107:LEU:HD13	1:A:188:ASN:ND2	2.32	0.45
1:B:423:VAL:H	1:B:427:TYR:C	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:MET:HE2	1:A:29:MET:HB3	1.86	0.45
1:A:102:PRO:O	1:A:103:ASP:CB	2.65	0.45
1:B:70:THR:HG23	1:B:73:ALA:H	1.82	0.45
1:B:98:GLY:HA3	1:B:109:TYR:CE2	2.52	0.44
1:B:209:TRP:HH2	1:B:370:TRP:CH2	2.35	0.44
1:B:248:HIS:CE1	1:B:313:ARG:NH1	2.86	0.44
1:A:183:MET:HE1	1:A:261:GLU:OE1	2.17	0.44
1:A:87:LEU:HD21	1:A:119:PHE:CD2	2.52	0.44
1:A:158:GLY:C	1:A:162:PHE:CE2	2.96	0.44
1:A:191:ILE:O	1:A:194:LEU:HB3	2.18	0.43
1:A:45:TYR:N	1:A:45:TYR:CD1	2.85	0.43
1:A:102:PRO:O	1:A:103:ASP:HB3	2.16	0.43
1:B:347:LEU:N	2:B:501:NDP:N1A	2.55	0.43
1:A:230:PRO:HG3	1:A:293:LEU:CD2	2.48	0.43
1:A:339:LYS:HB2	1:A:339:LYS:HE3	1.72	0.43
1:B:206:MET:HG3	1:B:275:LEU:CD2	2.48	0.43
1:B:323:ARG:NH2	1:B:345:LEU:O	2.47	0.43
1:A:188:ASN:OD1	1:A:188:ASN:N	2.50	0.43
1:B:53:THR:HB	1:B:55:ASP:H	1.84	0.43
1:A:107:LEU:CD1	1:A:190:ARG:HH21	2.32	0.43
1:A:203:ARG:HB2	1:A:204:PRO:HD3	2.01	0.43
1:B:243:ILE:HD12	1:B:243:ILE:HG23	1.76	0.43
1:A:99:MET:HG3	1:A:259:LYS:HD3	2.00	0.43
1:A:107:LEU:HD23	1:A:108:ASP:C	2.43	0.42
1:A:130:MET:C	1:A:132:TRP:H	2.26	0.42
1:A:423:VAL:CG2	1:A:427:TYR:N	2.82	0.42
1:B:59:TRP:CE3	1:B:59:TRP:HA	2.54	0.42
1:B:141:GLN:O	1:B:145:LEU:HG	2.20	0.42
1:B:197:LYS:NZ	1:B:261:GLU:O	2.35	0.42
1:A:190:ARG:HG2	1:A:195:ASP:HA	2.01	0.42
1:A:196:LEU:CB	1:A:263:PHE:HE2	2.33	0.42
1:A:99:MET:HG3	1:A:259:LYS:CD	2.50	0.42
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.45	0.42
1:A:124:VAL:HG11	1:A:211:LEU:HD22	2.01	0.42
1:B:91:ALA:CB	1:B:112:ASN:HB3	2.49	0.42
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.92	0.42
1:B:339:LYS:HB2	1:B:339:LYS:HE3	1.76	0.41
1:A:91:ALA:O	1:A:110:ARG:NH2	2.53	0.41
1:A:347:LEU:HD23	1:A:352:TRP:CD1	2.55	0.41
1:B:242:LEU:O	1:B:245:TYR:HB3	2.20	0.41
1:B:333:LYS:CG	1:B:334:PRO:CD	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:ND2	1:A:238:GLN:OE1	2.53	0.41
1:B:87:LEU:O	1:B:91:ALA:HB2	2.20	0.41
1:B:95:THR:HA	1:B:110:ARG:HA	2.02	0.41
1:B:179:TYR:C	1:B:181:TYR:N	2.77	0.41
1:B:203:ARG:HB2	1:B:204:PRO:HD3	2.02	0.41
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.84	0.41
1:B:256:TRP:CE2	1:B:398:ARG:HD2	2.55	0.41
1:B:423:VAL:HB	1:B:427:TYR:H	1.85	0.41
1:B:380:ILE:HB	1:B:381:PRO:HD3	2.01	0.41
1:A:357:HIS:N	1:A:421:ARG:O	2.54	0.41
1:B:45:TYR:CD2	1:B:65:HIS:CD2	3.08	0.41
1:B:134:ASP:OD1	1:B:134:ASP:N	2.54	0.41
1:B:151:ILE:O	1:B:155:VAL:HG12	2.20	0.41
1:B:204:PRO:O	1:B:208:PHE:HB2	2.20	0.41
1:A:317:ILE:HG22	1:A:321:HIS:CD2	2.56	0.41
1:A:145:LEU:HD13	1:A:208:PHE:HZ	1.86	0.41
1:A:216:MET:HE3	1:A:216:MET:HB2	1.83	0.41
1:A:252:VAL:O	1:A:258:ILE:HG13	2.20	0.41
1:B:231:MET:HE1	1:B:283:ALA:CB	2.51	0.41
1:A:329:ILE:H	1:A:329:ILE:HG13	1.58	0.41
1:B:234:VAL:HG23	1:B:373:PRO:HG2	2.02	0.41
1:B:421:ARG:C	1:B:422:ILE:HG13	2.46	0.40
1:A:344:SER:HB2	1:A:407:TYR:HE1	1.86	0.40
1:A:103:ASP:CG	1:A:105:SER:HB2	2.46	0.40
1:A:275:LEU:HD12	1:A:279:TYR:CE2	2.56	0.40
1:A:321:HIS:NE2	1:B:226:THR:CG2	2.79	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	389/427 (91%)	353 (91%)	36 (9%)	0	100	100
1	B	385/427 (90%)	349 (91%)	36 (9%)	0	100	100
All	All	774/854 (91%)	702 (91%)	72 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	306/358 (86%)	273 (89%)	33 (11%)	6	11
1	B	327/358 (91%)	293 (90%)	34 (10%)	7	13
All	All	633/716 (88%)	566 (89%)	67 (11%)	6	12

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	92	PRO
1	A	100	LYS
1	A	110	ARG
1	A	112	ASN
1	A	120	THR
1	A	121	LEU
1	A	124	VAL
1	A	127	LEU
1	A	129	THR
1	A	134	ASP
1	A	146	LEU
1	A	163	TRP
1	A	187	LEU
1	A	196	LEU
1	A	206	MET
1	A	207	ILE
1	A	219	LYS

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Mol	Chain	Res	Type
1	A	227	VAL
1	A	229	VAL
1	A	263	PHE
1	A	267	LEU
1	A	275	LEU
1	A	281	LEU
1	A	282	GLN
1	A	284	GLN
1	A	287	VAL
1	A	293	LEU
1	A	295	VAL
1	A	329	ILE
1	A	333	LYS
1	A	337	TYR
1	A	380	ILE
1	B	30	ILE
1	B	42	CYS
1	B	50	LEU
1	B	120	THR
1	B	121	LEU
1	B	124	VAL
1	B	127	LEU
1	B	129	THR
1	B	134	ASP
1	B	151	ILE
1	B	187	LEU
1	B	201	GLU
1	B	206	MET
1	B	207	ILE
1	B	216	MET
1	B	222	GLU
1	B	229	VAL
1	B	250	GLU
1	B	267	LEU
1	B	280	THR
1	B	281	LEU
1	B	284	GLN
1	B	288	HIS
1	B	295	VAL
1	B	306	LEU
1	B	317	ILE
1	B	329	ILE

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Mol	Chain	Res	Type
1	B	333	LYS
1	B	337	TYR
1	B	347	LEU
1	B	380	ILE
1	B	385	ILE
1	B	416	LYS
1	B	425	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	84	GLN
1	A	88	GLN
1	A	141	GLN
1	A	260	HIS
1	A	284	GLN
1	B	65	HIS
1	B	88	GLN
1	B	213	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NDP	A	501	-	32,33,52	1.56	4 (12%)	50,52,80	1.57	8 (16%)
2	NDP	B	501	-	32,33,52	1.55	6 (18%)	50,52,80	1.62	7 (14%)

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	NDP	A	501	-	-	7/21/37/77	0/3/3/5
2	NDP	B	501	-	-	9/21/37/77	0/3/3/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NDP	C5A-C4A	5.67	1.49	1.39
2	B	501	NDP	C5A-C4A	5.30	1.48	1.39
2	B	501	NDP	C8A-N7A	3.41	1.38	1.31
2	A	501	NDP	C8A-N7A	3.20	1.37	1.31
2	A	501	NDP	C5A-C6A	2.79	1.48	1.41
2	B	501	NDP	C5A-C6A	2.48	1.47	1.41
2	A	501	NDP	PA-O3	2.31	1.62	1.59
2	B	501	NDP	C5A-N7A	-2.23	1.35	1.39
2	B	501	NDP	P2B-O2B	2.18	1.63	1.59
2	B	501	NDP	PA-O3	2.11	1.61	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NDP	C5A-C4A-N3A	-5.76	118.78	126.72
2	A	501	NDP	C5A-C4A-N3A	-5.48	119.17	126.72
2	B	501	NDP	N3A-C4A-N9A	4.22	134.34	127.17
2	A	501	NDP	N3A-C4A-N9A	3.96	133.89	127.17
2	B	501	NDP	C2A-N3A-C4A	3.84	121.20	111.83
2	B	501	NDP	N3A-C2A-N1A	-3.57	123.17	128.58
2	A	501	NDP	C2A-N3A-C4A	3.43	120.21	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NDP	N3A-C2A-N1A	-2.75	124.41	128.58
2	A	501	NDP	O2B-C2B-C3B	-2.66	102.15	111.68
2	B	501	NDP	C4A-C5A-N7A	-2.63	107.57	110.58
2	B	501	NDP	O2N-PN-O1N	2.57	120.85	110.83
2	A	501	NDP	O2N-PN-O1N	2.57	120.84	110.83
2	A	501	NDP	C4A-C5A-N7A	-2.36	107.88	110.58
2	B	501	NDP	O2B-C2B-C3B	-2.20	103.79	111.68
2	A	501	NDP	O4B-C1B-C2B	-2.14	102.91	106.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C3B-C4B-C5B-O5B
2	B	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	C3B-C4B-C5B-O5B
2	A	501	NDP	C3B-C2B-O2B-P2B
2	B	501	NDP	C3B-C2B-O2B-P2B
2	A	501	NDP	PN-O3-PA-O5B
2	B	501	NDP	PA-O3-PN-O1N
2	B	501	NDP	PA-O3-PN-O2N
2	A	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5B-O5B-PA-O1A
2	A	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	C1B-C2B-O2B-P2B
2	A	501	NDP	C1B-C2B-O2B-P2B
2	B	501	NDP	PA-O3-PN-O5D

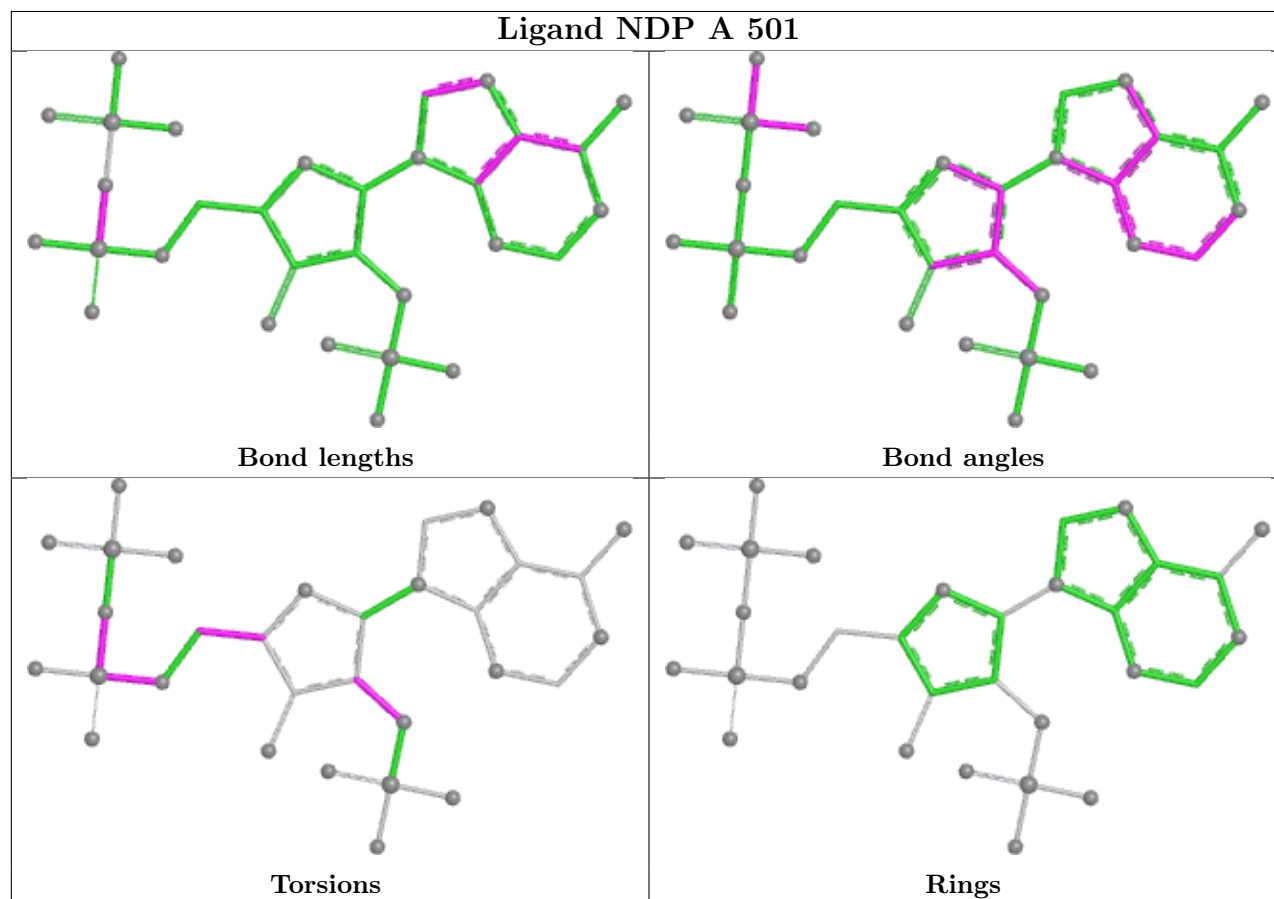
There are no ring outliers.

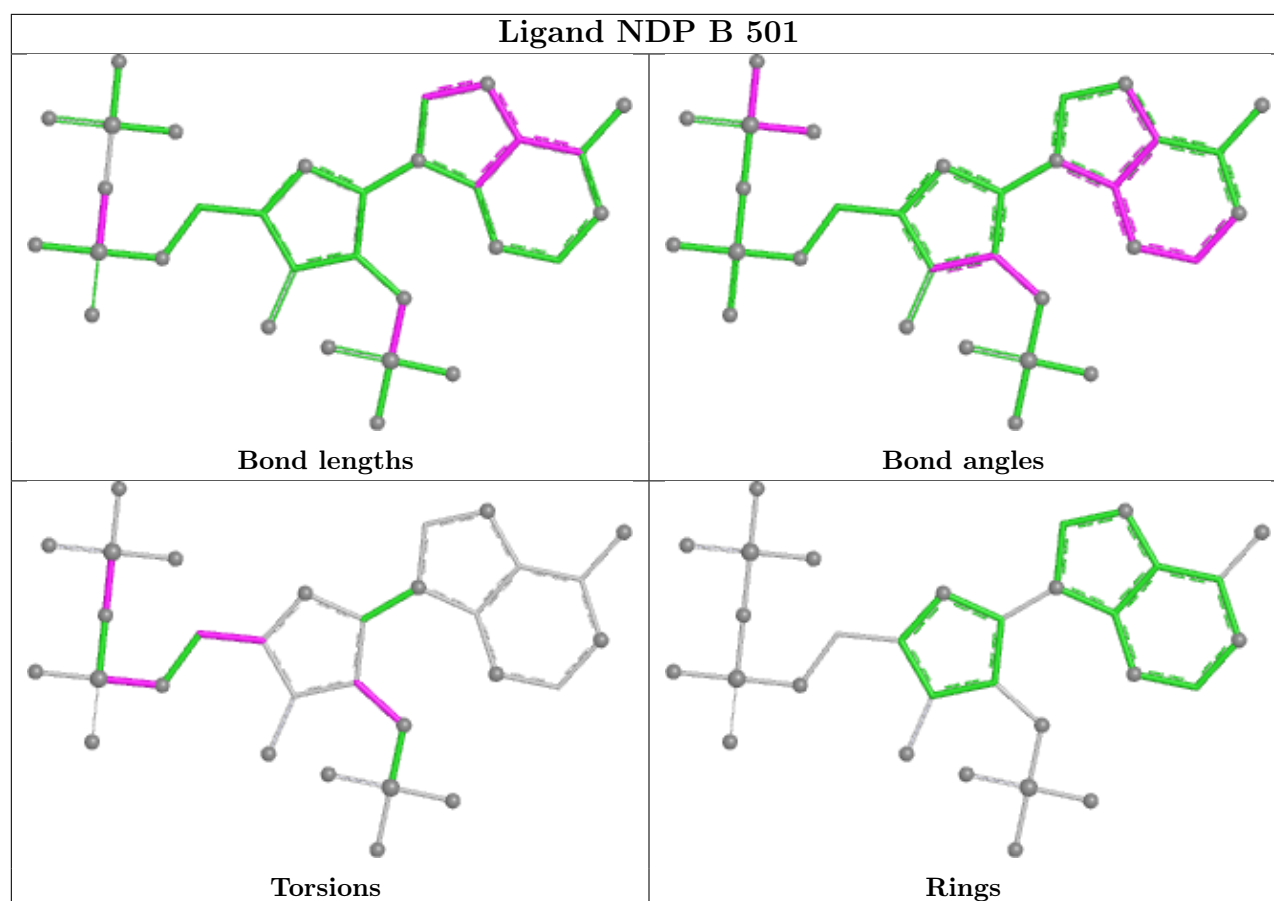
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	2	0
2	B	501	NDP	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 than 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.





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	393/427 (92%)	1.07	67 (17%) 4 4	47, 86, 148, 227	0
1	B	389/427 (91%)	0.93	53 (13%) 7 6	42, 82, 139, 239	0
All	All	782/854 (91%)	1.00	120 (15%) 5 5	42, 84, 145, 239	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	PRO	9.7
1	A	162	PHE	7.8
1	A	186	ALA	6.8
1	A	185	THR	6.4
1	A	327	ASN	6.4
1	A	180	ASP	6.2
1	B	327	ASN	5.4
1	A	424	PRO	5.3
1	A	100	LYS	5.1
1	B	185	THR	5.0
1	A	187	LEU	4.9
1	A	101	LEU	4.8
1	B	26	LEU	4.8
1	A	423	VAL	4.7
1	A	178	PHE	4.5
1	B	105	SER	4.4
1	A	263	PHE	4.4
1	B	263	PHE	4.3
1	A	66	VAL	4.2
1	B	342	GLN	4.0
1	A	341	LYS	4.0
1	B	112	ASN	4.0
1	B	292	ASP	3.8
1	A	164	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	GLY	3.6
1	B	187	LEU	3.6
1	A	325	ASP	3.5
1	A	177	PRO	3.5
1	A	23	PHE	3.5
1	A	207	ILE	3.4
1	B	143	GLY	3.4
1	A	72	HIS	3.4
1	A	61	ARG	3.4
1	A	54	SER	3.4
1	A	184	GLY	3.4
1	B	178	PHE	3.4
1	B	226	THR	3.3
1	A	262	LYS	3.3
1	A	426	ILE	3.3
1	B	25	TRP	3.3
1	A	26	LEU	3.2
1	B	261	GLU	3.2
1	A	334	PRO	3.2
1	B	341	LYS	3.2
1	A	83	GLY	3.2
1	A	279	TYR	3.2
1	A	397	LYS	3.1
1	B	264	GLY	3.1
1	A	59	TRP	3.1
1	A	257	ASP	3.0
1	A	104	GLY	3.0
1	A	160	LEU	3.0
1	A	256	TRP	3.0
1	A	383	PHE	3.0
1	B	179	TYR	2.9
1	B	321	HIS	2.9
1	A	288	HIS	2.9
1	A	159	PHE	2.8
1	B	72	HIS	2.8
1	B	288	HIS	2.8
1	B	328	ARG	2.8
1	B	101	LEU	2.7
1	B	256	TRP	2.7
1	A	261	GLU	2.7
1	A	250	GLU	2.7
1	B	193	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	196	LEU	2.6
1	A	293	LEU	2.6
1	B	158	GLY	2.6
1	B	100	LYS	2.6
1	B	67	ALA	2.6
1	B	103	ASP	2.5
1	B	93	GLY	2.5
1	B	58	ALA	2.5
1	B	157	ALA	2.5
1	B	182	PHE	2.5
1	B	177	PRO	2.5
1	B	109	TYR	2.5
1	A	163	TRP	2.4
1	B	257	ASP	2.4
1	B	352	TRP	2.4
1	B	186	ALA	2.4
1	B	60	ARG	2.4
1	B	110	ARG	2.4
1	A	188	ASN	2.4
1	A	333	LYS	2.4
1	B	290	THR	2.4
1	B	92	PRO	2.4
1	A	161	TYR	2.3
1	A	375	ALA	2.3
1	A	399	ASP	2.3
1	A	60	ARG	2.3
1	A	404	LEU	2.3
1	A	405	ALA	2.3
1	A	292	ASP	2.3
1	B	99	MET	2.3
1	B	417	LYS	2.3
1	A	395	ARG	2.3
1	A	25	TRP	2.3
1	A	370	TRP	2.3
1	A	269	TRP	2.2
1	A	335	ALA	2.2
1	A	65	HIS	2.2
1	B	335	ALA	2.2
1	A	328	ARG	2.2
1	A	94	PRO	2.2
1	A	99	MET	2.2
1	B	94	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	181	TYR	2.1
1	B	55	ASP	2.1
1	A	24	SER	2.1
1	B	54	SER	2.1
1	B	267	LEU	2.1
1	A	89	VAL	2.1
1	B	395	ARG	2.0
1	A	411	TRP	2.0
1	A	45	TYR	2.0
1	B	397	LYS	2.0
1	B	411	TRP	2.0
1	B	106	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

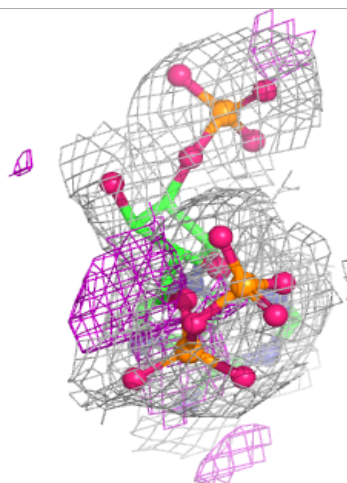
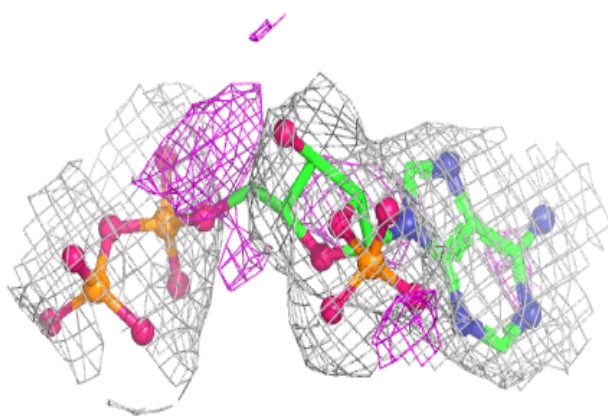
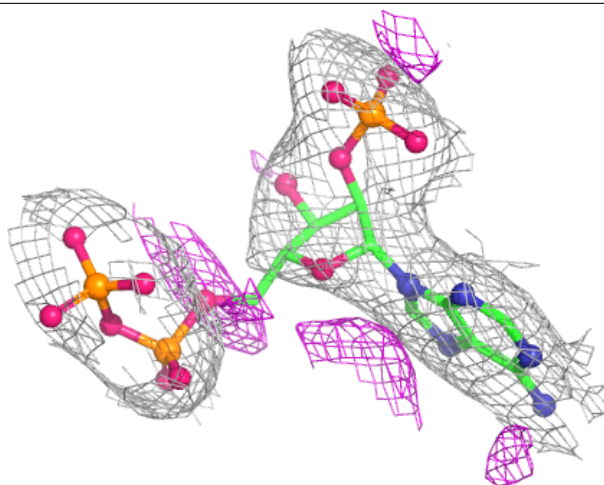
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	B	501	31/48	0.87	0.12	46,89,114,364	0
2	NDP	A	501	31/48	0.89	0.13	41,77,119,301	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.

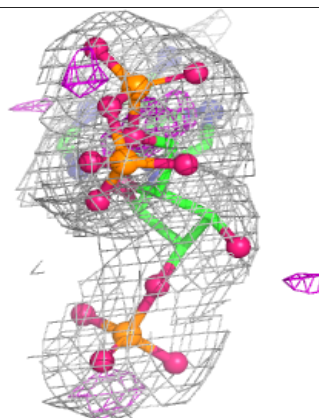
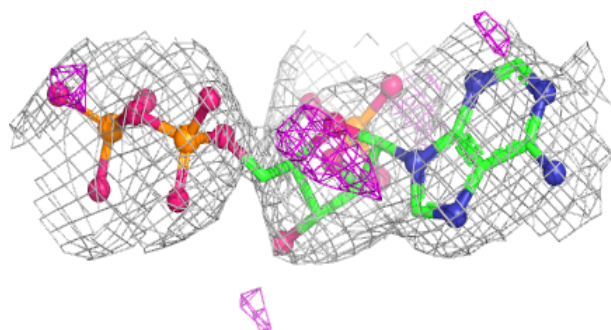
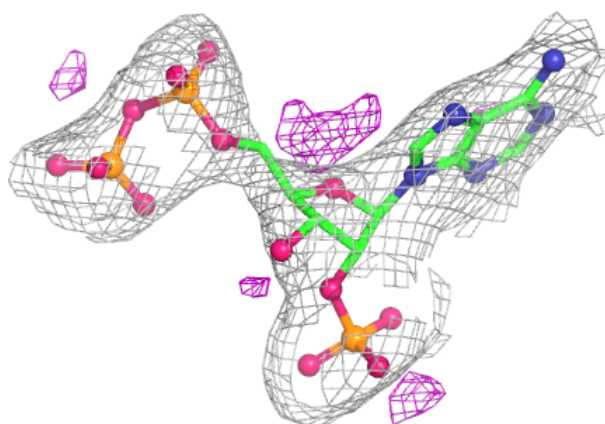
Electron density around NDP B 501:

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



Electron density around NDP A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.