



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:14 PM UTC

PDB ID : 2EGH / pdb_00002egh
Title : Crystal structure of 1-deoxy-D-xylulose 5-phosphate reductoisomerase complexed with a magnesium ion, NADPH and fosmidomycin
Authors : Yajima, S.; Hara, K.; Iino, D.; Sasaki, Y.; Kuzuyama, T.; Seto, H.
Deposited on : 2007-03-01
Resolution : 2.20 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

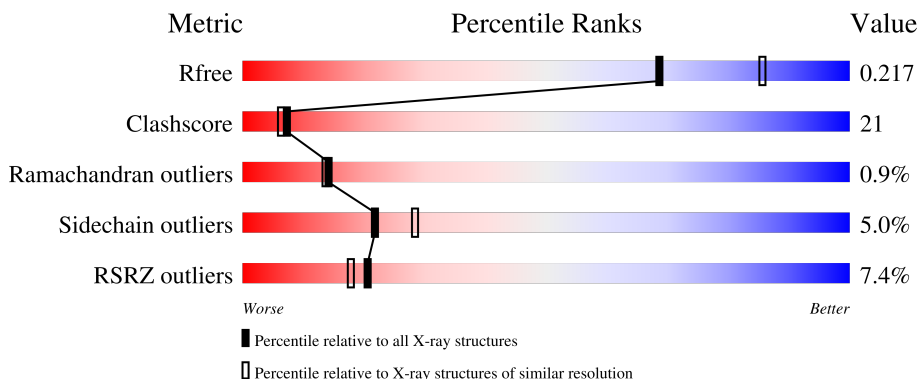
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	424	8% 58% 33% • 6%
1	B	424	6% 61% 29% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6482 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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3036	1895	536	579	26			
1	B	398	Total	C	N	O	S	0	0	0
			3025	1889	534	576	26			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	cloning artifact	UNP P45568
A	-9	ARG	-	cloning artifact	UNP P45568
A	-8	GLY	-	cloning artifact	UNP P45568
A	-7	SER	-	cloning artifact	UNP P45568
A	-6	HIS	-	cloning artifact	UNP P45568
A	-5	HIS	-	cloning artifact	UNP P45568
A	-4	HIS	-	cloning artifact	UNP P45568
A	-3	HIS	-	cloning artifact	UNP P45568
A	-2	HIS	-	cloning artifact	UNP P45568
A	-1	HIS	-	cloning artifact	UNP P45568
A	0	GLY	-	cloning artifact	UNP P45568
A	398	SER	-	cloning artifact	UNP P45568
A	399	ALA	-	cloning artifact	UNP P45568
A	400	CYS	-	cloning artifact	UNP P45568
A	401	ASP	-	cloning artifact	UNP P45568
A	402	LEU	-	cloning artifact	UNP P45568
A	403	GLY	-	cloning artifact	UNP P45568
A	404	THR	-	cloning artifact	UNP P45568
A	405	PRO	-	cloning artifact	UNP P45568
A	406	GLY	-	cloning artifact	UNP P45568
A	407	ARG	-	cloning artifact	UNP P45568
A	408	PRO	-	cloning artifact	UNP P45568
A	409	ALA	-	cloning artifact	UNP P45568
A	410	ALA	-	cloning artifact	UNP P45568
A	411	LYS	-	cloning artifact	UNP P45568

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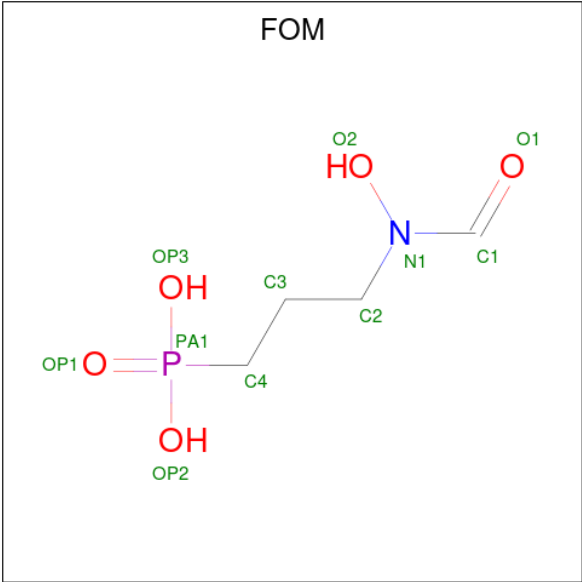
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Chain	Residue	Modelled	Actual	Comment	Reference
A	412	LEU	-	cloning artifact	UNP P45568
A	413	ASN	-	cloning artifact	UNP P45568
B	-10	MET	-	cloning artifact	UNP P45568
B	-9	ARG	-	cloning artifact	UNP P45568
B	-8	GLY	-	cloning artifact	UNP P45568
B	-7	SER	-	cloning artifact	UNP P45568
B	-6	HIS	-	cloning artifact	UNP P45568
B	-5	HIS	-	cloning artifact	UNP P45568
B	-4	HIS	-	cloning artifact	UNP P45568
B	-3	HIS	-	cloning artifact	UNP P45568
B	-2	HIS	-	cloning artifact	UNP P45568
B	-1	HIS	-	cloning artifact	UNP P45568
B	0	GLY	-	cloning artifact	UNP P45568
B	398	SER	-	cloning artifact	UNP P45568
B	399	ALA	-	cloning artifact	UNP P45568
B	400	CYS	-	cloning artifact	UNP P45568
B	401	ASP	-	cloning artifact	UNP P45568
B	402	LEU	-	cloning artifact	UNP P45568
B	403	GLY	-	cloning artifact	UNP P45568
B	404	THR	-	cloning artifact	UNP P45568
B	405	PRO	-	cloning artifact	UNP P45568
B	406	GLY	-	cloning artifact	UNP P45568
B	407	ARG	-	cloning artifact	UNP P45568
B	408	PRO	-	cloning artifact	UNP P45568
B	409	ALA	-	cloning artifact	UNP P45568
B	410	ALA	-	cloning artifact	UNP P45568
B	411	LYS	-	cloning artifact	UNP P45568
B	412	LEU	-	cloning artifact	UNP P45568
B	413	ASN	-	cloning artifact	UNP P45568

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

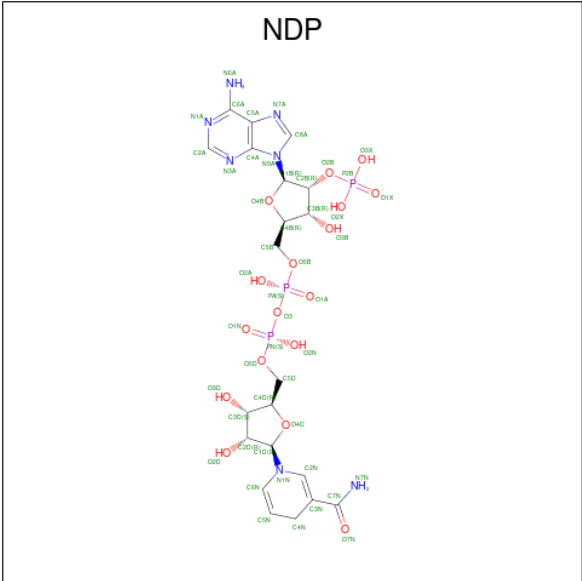
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (CCD ID: FOM) (formula: C₄H₁₀NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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

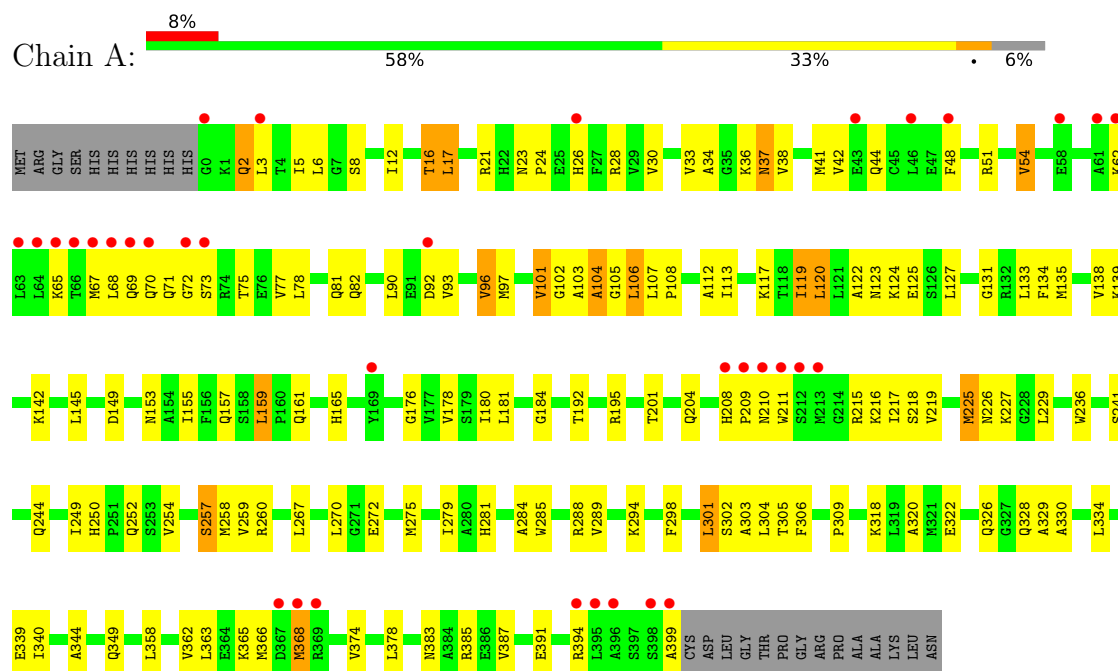
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		
5	B	151	Total	O	0	0
			151	151		

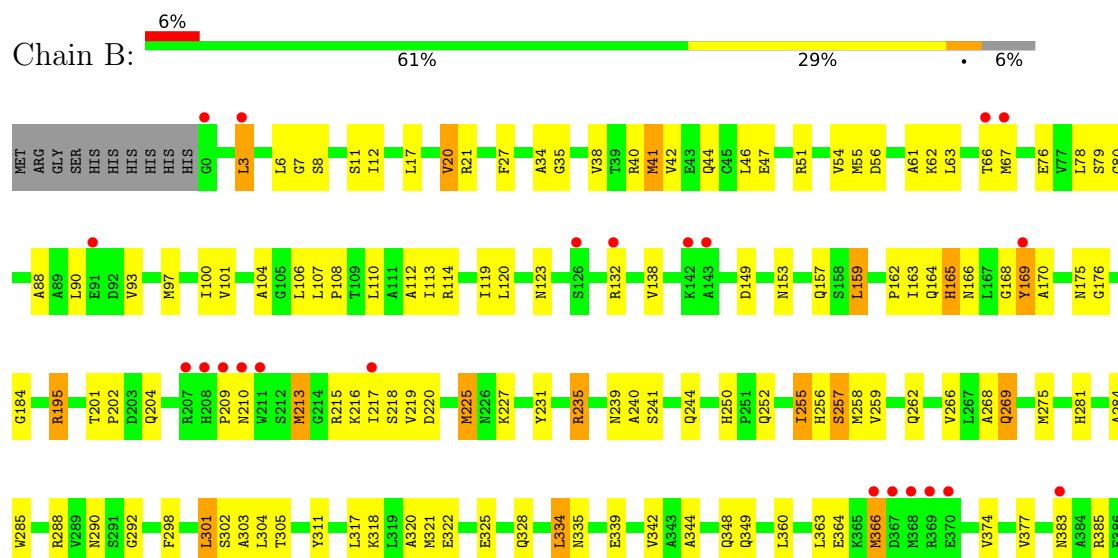
3 Residue-property plots [i](#)

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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



V387	A388	R389	F390	E391	E394	L395	A396	S397	SER	ALA	CYS	ASP	LEU	GLY	THR	PRO	GLY	ARG	PRO	ALA	ALA	LYS	LEU	ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.59Å 59.12Å 87.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.21 – 2.20 47.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.21-2.20) 98.3 (47.21-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.225 0.214 , 0.217	Depositor DCC
R_{free} test set	4474 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6482	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: MG, NDP, FOM

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	0.48	1/3084 (0.0%)	0.92	8/4181 (0.2%)
1	B	0.43	0/3073	0.92	7/4166 (0.2%)
All	All	0.46	1/6157 (0.0%)	0.92	15/8347 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ASN	C-N	10.25	1.46	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	HIS	N-CA-C	-8.84	96.26	110.32
1	B	225	MET	N-CA-C	-7.76	102.82	111.82
1	B	209	PRO	N-CA-C	-7.15	104.62	114.27
1	A	225	MET	N-CA-C	-6.93	103.78	111.82
1	A	302	SER	N-CA-C	-6.78	101.40	110.55
1	B	8	SER	N-CA-C	5.99	117.89	111.36
1	A	104	ALA	N-CA-C	-5.44	103.31	110.33
1	A	254	VAL	N-CA-C	-5.35	105.63	110.82
1	B	80	GLY	N-CA-C	5.35	118.28	112.29
1	B	255	ILE	N-CA-C	-5.29	101.90	108.89
1	B	302	SER	N-CA-C	-5.25	101.97	110.32
1	A	119	ILE	N-CA-C	5.15	115.27	107.80
1	A	101	VAL	N-CA-C	5.09	116.49	109.46
1	A	192	THR	N-CA-C	5.05	115.41	109.60
1	A	8	SER	N-CA-C	5.05	117.68	111.82

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	3036	0	3059	129	0
1	B	3025	0	3049	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	8	0	0
3	B	11	0	7	0	0
4	A	48	0	26	10	0
4	B	48	0	26	18	0
5	A	150	0	0	7	0
5	B	151	0	0	5	0
All	All	6482	0	6175	255	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 21.

All (255) 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:149:ASP:HA	4:B:3002:NDP:H5N	1.40	1.00
1:B:256:HIS:HD2	1:B:269:GLN:HE22	1.13	0.95
1:A:270:LEU:HD22	1:B:258:MET:HE1	1.51	0.93
1:B:256:HIS:CD2	1:B:269:GLN:HE22	1.91	0.87
1:B:275:MET:HE2	4:B:3002:NDP:H42N	1.57	0.85
1:B:123:ASN:HA	4:B:3002:NDP:O3D	1.79	0.83
1:A:123:ASN:HA	4:A:3001:NDP:O3D	1.81	0.81
1:B:7:GLY:CA	1:B:100:ILE:HD13	2.13	0.79
1:B:241:SER:H	1:B:244:GLN:HE21	1.30	0.79
1:A:12:ILE:O	1:A:16:THR:HG23	1.81	0.79
1:B:159:LEU:HD13	1:B:259:VAL:HG21	1.65	0.79
1:A:275:MET:HE2	4:A:3001:NDP:H42N	1.65	0.78
1:A:159:LEU:HD13	1:A:259:VAL:HG21	1.64	0.78
1:A:73:SER:OG	1:A:75:THR:HG22	1.83	0.77
1:B:201:THR:HG22	1:B:204:GLN:HG3	1.66	0.76
1:B:366:MET:HE3	1:B:383:ASN:ND2	2.01	0.76
1:A:101:VAL:HG22	1:A:102:GLY:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:HA	4:A:3001:NDP:H5N	1.68	0.75
1:A:107:LEU:HD21	1:A:374:VAL:HG21	1.68	0.74
1:A:249:ILE:HD11	1:A:309:PRO:HB3	1.70	0.72
1:A:303:ALA:HB1	1:B:303:ALA:HB1	1.74	0.70
1:A:33:VAL:HG22	1:A:54:VAL:HG13	1.73	0.69
1:A:184:GLY:HA3	1:A:227:LYS:HE3	1.74	0.69
1:A:155:ILE:HD12	1:A:180:ILE:HG23	1.75	0.68
1:B:275:MET:CE	4:B:3002:NDP:H42N	2.23	0.68
1:A:252:GLN:HE22	1:A:305:THR:H	1.40	0.68
1:B:195:ARG:HH11	1:B:195:ARG:HB3	1.60	0.67
1:A:241:SER:H	1:A:244:GLN:HE21	1.40	0.66
1:A:344:ALA:HA	1:A:349:GLN:HE21	1.61	0.66
1:B:113:ILE:HD12	1:B:138:VAL:HG22	1.79	0.65
1:B:166:ASN:HA	1:B:169:TYR:CZ	2.31	0.65
1:B:7:GLY:HA3	1:B:100:ILE:HD13	1.78	0.65
1:A:298:PHE:HA	1:A:301:LEU:HD22	1.79	0.64
1:B:201:THR:HG22	1:B:204:GLN:CG	2.27	0.64
1:A:33:VAL:HG22	1:A:54:VAL:CG1	2.27	0.63
1:A:249:ILE:CD1	1:A:309:PRO:HB3	2.28	0.62
1:B:252:GLN:HE22	1:B:305:THR:H	1.45	0.62
1:B:21:ARG:HD3	1:B:47:GLU:OE2	2.00	0.62
1:B:100:ILE:HD12	4:B:3002:NDP:N3A	2.15	0.62
1:B:164:GLN:NE2	1:B:285:TRP:HE1	1.98	0.61
1:B:298:PHE:HA	1:B:301:LEU:HD22	1.81	0.61
1:A:134:PHE:O	1:A:138:VAL:HG13	2.00	0.61
1:B:275:MET:HG3	4:B:3002:NDP:O7N	2.01	0.61
1:B:63:LEU:O	1:B:67:MET:HG2	2.01	0.61
1:B:252:GLN:NE2	1:B:305:THR:H	1.99	0.60
1:B:201:THR:HG23	1:B:204:GLN:H	1.65	0.60
1:B:255:ILE:HD11	1:B:304:LEU:HD13	1.83	0.60
1:B:3:LEU:HD21	1:B:27:PHE:HB3	1.83	0.59
1:A:101:VAL:CG2	1:A:102:GLY:N	2.64	0.59
1:A:195:ARG:HG3	5:A:3073:HOH:O	2.01	0.59
1:A:225:MET:HE1	1:A:320:ALA:HB2	1.85	0.59
1:B:7:GLY:CA	1:B:100:ILE:CD1	2.80	0.58
1:B:217:ILE:HD12	1:B:217:ILE:H	1.68	0.58
1:A:252:GLN:NE2	1:A:305:THR:H	2.01	0.58
1:B:54:VAL:HG22	1:B:78:LEU:HB2	1.86	0.57
1:A:101:VAL:HG23	4:A:3001:NDP:H3D	1.86	0.57
1:A:135:MET:HE1	1:A:145:LEU:CD1	2.35	0.57
1:B:162:PRO:HB2	1:B:175:ASN:ND2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD13	1:A:122:ALA:HB1	1.87	0.57
1:B:387:VAL:O	1:B:391:GLU:HG2	2.04	0.56
1:B:162:PRO:HB2	1:B:175:ASN:HD21	1.69	0.56
1:A:122:ALA:O	4:A:3001:NDP:O4D	2.23	0.56
1:A:181:LEU:HD23	1:A:258:MET:HE3	1.87	0.56
1:A:90:LEU:O	1:A:117:LYS:HE3	2.05	0.56
1:B:41:MET:HG3	1:B:55:MET:SD	2.45	0.56
1:B:100:ILE:HD12	4:B:3002:NDP:C4A	2.35	0.56
1:B:149:ASP:CA	4:B:3002:NDP:H5N	2.25	0.56
1:B:395:LEU:O	1:B:395:LEU:HD13	2.04	0.56
1:A:123:ASN:CA	4:A:3001:NDP:O3D	2.54	0.56
1:A:2:GLN:HB3	1:A:93:VAL:HA	1.86	0.56
1:B:184:GLY:HA3	1:B:227:LYS:HE3	1.87	0.56
1:B:255:ILE:CD1	1:B:304:LEU:HD13	2.36	0.56
1:B:258:MET:HG2	1:B:268:ALA:HB2	1.86	0.56
1:A:102:GLY:C	1:A:125:GLU:HG3	2.31	0.55
1:A:67:MET:O	1:A:71:GLN:HG2	2.06	0.55
1:A:101:VAL:CG2	4:A:3001:NDP:H3D	2.35	0.55
1:B:40:ARG:O	1:B:44:GLN:HG3	2.06	0.55
1:A:329:ALA:HB3	1:A:368:MET:HG3	1.89	0.55
1:A:161:GLN:HG3	1:A:165:HIS:HD2	1.72	0.55
1:B:344:ALA:HA	1:B:349:GLN:HE21	1.70	0.55
1:A:362:VAL:O	1:A:366:MET:HG2	2.07	0.54
1:A:102:GLY:CA	1:A:125:GLU:HG3	2.38	0.54
1:B:216:LYS:HD2	1:B:342:VAL:HG11	1.89	0.54
1:B:225:MET:HE1	1:B:320:ALA:HB2	1.89	0.54
1:B:166:ASN:HA	1:B:169:TYR:CE1	2.43	0.54
1:B:235:ARG:NH2	1:B:325:GLU:OE2	2.41	0.54
1:A:23:ASN:HB3	1:A:26:HIS:CD2	2.43	0.54
1:B:7:GLY:N	1:B:100:ILE:CD1	2.70	0.54
1:A:105:GLY:C	1:A:108:PRO:HD2	2.33	0.54
1:B:318:LYS:O	1:B:322:GLU:HG3	2.07	0.53
1:B:107:LEU:N	1:B:107:LEU:HD22	2.24	0.53
1:A:3:LEU:HD12	1:A:5:ILE:HD11	1.90	0.53
1:A:340:ILE:HD11	1:A:385:ARG:HG2	1.90	0.53
1:A:107:LEU:CD2	1:A:374:VAL:HG21	2.39	0.53
1:A:62:LYS:O	1:A:65:LYS:HB3	2.09	0.53
1:A:155:ILE:HD11	1:A:257:SER:HB3	1.91	0.53
1:A:288:ARG:HB2	1:B:176:GLY:HA3	1.90	0.53
1:A:101:VAL:CG2	1:A:102:GLY:H	2.22	0.53
1:B:153:ASN:ND2	1:B:157:GLN:HE21	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLY:O	1:B:239:ASN:HB2	2.09	0.52
1:A:12:ILE:O	1:A:16:THR:CG2	2.55	0.52
1:A:155:ILE:CD1	1:A:257:SER:HB3	2.39	0.52
1:A:101:VAL:HG22	1:A:102:GLY:H	1.72	0.52
1:A:103:ALA:O	1:A:106:LEU:HB2	2.10	0.52
1:B:258:MET:HE2	1:B:266:VAL:HG12	1.92	0.52
1:A:241:SER:H	1:A:244:GLN:NE2	2.06	0.51
1:B:213:MET:HE3	1:B:218:SER:HA	1.92	0.51
1:A:36:LYS:O	1:A:38:VAL:N	2.42	0.51
1:A:394:ARG:HG2	1:A:399:ALA:HB3	1.92	0.51
1:A:96:VAL:HG11	1:A:112:ALA:HB1	1.90	0.51
1:B:164:GLN:HE22	1:B:285:TRP:HE1	1.58	0.51
1:A:340:ILE:HD11	1:A:385:ARG:CG	2.42	0.50
1:B:90:LEU:O	1:B:93:VAL:HG22	2.11	0.50
1:B:101:VAL:HG23	4:B:3002:NDP:H3D	1.92	0.50
1:B:104:ALA:HB1	4:B:3002:NDP:N6A	2.26	0.50
1:B:7:GLY:N	1:B:100:ILE:HD11	2.27	0.49
1:B:195:ARG:H	1:B:195:ARG:NH1	2.10	0.49
1:B:290:ASN:ND2	1:B:292:GLY:H	2.09	0.49
1:B:256:HIS:HE1	5:B:3016:HOH:O	1.94	0.49
1:A:3:LEU:H	1:A:3:LEU:HD23	1.78	0.49
1:A:215:ARG:O	1:A:219:VAL:HG23	2.13	0.49
1:B:201:THR:CG2	1:B:204:GLN:H	2.26	0.49
1:B:215:ARG:HD3	5:B:3078:HOH:O	2.13	0.49
1:A:3:LEU:HD23	1:A:3:LEU:N	2.28	0.49
1:B:217:ILE:HD12	1:B:217:ILE:N	2.27	0.48
1:B:201:THR:CG2	1:B:204:GLN:HG3	2.39	0.48
1:A:2:GLN:HG3	1:A:30:VAL:CG2	2.43	0.48
1:A:217:ILE:HG12	5:A:3079:HOH:O	2.13	0.48
1:B:252:GLN:NE2	1:B:252:GLN:H	2.11	0.48
1:A:23:ASN:HB3	1:A:26:HIS:HD2	1.78	0.48
1:B:17:LEU:HA	1:B:20:VAL:HG13	1.96	0.48
1:B:258:MET:HG2	1:B:268:ALA:CB	2.43	0.48
1:A:133:LEU:H	1:A:328:GLN:HE22	1.62	0.47
1:B:216:LYS:HE2	1:B:220:ASP:OD1	2.14	0.47
1:B:112:ALA:HB1	1:B:119:ILE:HD11	1.95	0.47
1:B:114:ARG:HG3	1:B:114:ARG:HH11	1.79	0.47
1:A:3:LEU:CD1	1:A:5:ILE:HD11	2.45	0.47
1:B:97:MET:HE2	1:B:120:LEU:HD23	1.96	0.47
1:B:97:MET:HA	1:B:120:LEU:HB2	1.97	0.47
1:B:132:ARG:HB3	1:B:328:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:C	1:A:72:GLY:H	2.21	0.47
1:B:385:ARG:O	1:B:389:ARG:HG3	2.15	0.47
1:B:275:MET:CG	4:B:3002:NDP:O7N	2.63	0.47
1:B:61:ALA:CB	1:B:79:SER:HB3	2.44	0.47
1:A:77:VAL:O	1:A:78:LEU:HD23	2.15	0.46
1:A:153:ASN:HD21	1:A:281:HIS:CD2	2.34	0.46
1:B:35:GLY:H	4:B:3002:NDP:P2B	2.38	0.46
1:B:157:GLN:HG2	1:B:281:HIS:CE1	2.51	0.46
1:A:16:THR:HG21	1:A:97:MET:HG2	1.97	0.46
1:A:178:VAL:CG2	1:A:260:ARG:HD2	2.46	0.46
1:B:107:LEU:HD22	1:B:107:LEU:H	1.80	0.46
1:B:256:HIS:CD2	1:B:269:GLN:NE2	2.73	0.46
1:A:102:GLY:O	1:A:104:ALA:O	2.33	0.46
1:B:153:ASN:HD21	1:B:157:GLN:HE21	1.62	0.46
1:A:272:GLU:OE2	1:A:294:LYS:HE3	2.16	0.46
1:B:284:ALA:O	1:B:285:TRP:C	2.59	0.46
1:A:135:MET:O	1:A:138:VAL:HG22	2.16	0.46
1:A:225:MET:HE2	1:A:229:LEU:HG	1.98	0.46
1:A:270:LEU:N	1:A:270:LEU:HD12	2.31	0.46
1:B:241:SER:H	1:B:244:GLN:NE2	2.05	0.46
1:B:112:ALA:HB1	1:B:119:ILE:CD1	2.46	0.46
1:B:215:ARG:O	1:B:219:VAL:HG23	2.16	0.45
1:B:334:LEU:HG	1:B:363:LEU:HD11	1.98	0.45
1:A:127:LEU:HD11	1:A:135:MET:CE	2.47	0.45
1:A:157:GLN:HG2	1:A:281:HIS:CE1	2.52	0.45
1:B:258:MET:HE3	1:B:268:ALA:HB2	1.98	0.45
1:B:348:GLN:HA	5:B:3074:HOH:O	2.17	0.45
1:A:124:LYS:HE2	1:A:226:ASN:ND2	2.32	0.45
1:A:123:ASN:CB	4:A:3001:NDP:O3D	2.64	0.45
1:A:96:VAL:HG11	1:A:112:ALA:CB	2.47	0.45
1:B:12:ILE:HD11	4:B:3002:NDP:C7N	2.47	0.45
1:B:360:LEU:O	1:B:364:GLU:HG3	2.16	0.45
1:A:131:GLY:HA3	1:A:236:TRP:CD1	2.52	0.45
1:B:100:ILE:CD1	4:B:3002:NDP:N3A	2.80	0.45
1:B:288:ARG:NE	5:B:3109:HOH:O	2.21	0.45
1:A:17:LEU:HG	1:A:48:PHE:CZ	2.52	0.44
1:A:374:VAL:O	1:A:378:LEU:HG	2.18	0.44
1:A:250:HIS:CE1	1:A:252:GLN:HE21	2.35	0.44
1:B:11:SER:HB3	4:B:3002:NDP:O1N	2.17	0.44
1:A:97:MET:HA	1:A:120:LEU:HB2	2.00	0.44
1:B:7:GLY:N	1:B:100:ILE:HD13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:O	1:B:42:VAL:HG23	2.18	0.44
1:A:3:LEU:HD23	1:A:28:ARG:O	2.17	0.44
1:A:16:THR:HG21	1:A:97:MET:HE3	1.99	0.44
1:A:51:ARG:HG3	1:A:51:ARG:HH11	1.81	0.44
1:B:374:VAL:O	1:B:377:VAL:HG22	2.17	0.44
1:A:178:VAL:HG21	1:A:260:ARG:HD2	1.99	0.44
1:A:161:GLN:HG3	1:A:165:HIS:CD2	2.52	0.44
1:A:365:LYS:HE2	1:A:391:GLU:OE2	2.18	0.44
1:B:149:ASP:HA	4:B:3002:NDP:C5N	2.29	0.43
1:B:288:ARG:NH2	5:B:3109:HOH:O	2.51	0.43
1:A:81:GLN:HG3	5:A:3036:HOH:O	2.18	0.43
1:B:163:ILE:HD13	1:B:170:ALA:CB	2.49	0.43
1:A:281:HIS:HE1	5:A:3002:HOH:O	2.01	0.43
1:A:284:ALA:O	1:A:285:TRP:C	2.61	0.43
1:A:326:GLN:HB2	1:A:330:ALA:CB	2.48	0.43
1:A:82:GLN:HB2	5:A:3034:HOH:O	2.18	0.43
1:B:339:GLU:OE1	1:B:385:ARG:NH2	2.39	0.43
1:B:113:ILE:CD1	1:B:119:ILE:HG13	2.49	0.43
1:B:176:GLY:HA2	1:B:262:GLN:NE2	2.34	0.43
1:A:44:GLN:O	1:A:48:PHE:HD1	2.01	0.42
1:A:304:LEU:HB2	1:B:304:LEU:HB2	2.01	0.42
1:B:250:HIS:CE1	1:B:252:GLN:HE21	2.37	0.42
1:A:16:THR:CG2	1:A:97:MET:HE3	2.49	0.42
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.92	0.42
1:A:208:HIS:CD2	1:A:218:SER:OG	2.72	0.42
1:B:258:MET:HE2	1:B:266:VAL:CG1	2.50	0.42
1:A:70:GLN:C	1:A:72:GLY:N	2.76	0.42
1:A:176:GLY:HA3	1:B:288:ARG:HB2	2.01	0.42
1:B:366:MET:HE3	1:B:383:ASN:HD22	1.83	0.42
1:A:139:LYS:O	1:A:142:LYS:HD2	2.19	0.42
1:A:211:TRP:HZ3	1:A:275:MET:SD	2.43	0.42
1:A:318:LYS:HE3	1:A:322:GLU:OE1	2.18	0.42
1:B:317:LEU:O	1:B:321:MET:HG3	2.19	0.42
1:A:21:ARG:O	1:A:24:PRO:HD3	2.19	0.42
1:A:216:LYS:O	1:A:216:LYS:HD3	2.19	0.42
1:B:107:LEU:HB2	1:B:108:PRO:HD3	2.02	0.42
1:B:132:ARG:HB3	1:B:328:GLN:HE22	1.85	0.42
1:A:77:VAL:C	1:A:78:LEU:HD23	2.45	0.42
1:A:270:LEU:HD22	1:B:258:MET:CE	2.36	0.42
1:A:68:LEU:HD13	1:A:75:THR:CG2	2.50	0.42
1:B:62:LYS:O	1:B:66:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ALA:HB2	1:B:79:SER:HB3	2.01	0.41
1:B:88:ALA:HB1	1:B:112:ALA:HB2	2.01	0.41
1:A:16:THR:HA	1:A:279:ILE:HG21	2.01	0.41
1:A:135:MET:HE1	1:A:145:LEU:HD11	2.02	0.41
1:B:34:ALA:HB1	4:B:3002:NDP:O2X	2.20	0.41
1:B:123:ASN:CA	4:B:3002:NDP:O3D	2.61	0.41
1:A:12:ILE:HD11	4:A:3001:NDP:C2N	2.50	0.41
1:A:101:VAL:HB	4:A:3001:NDP:H51N	2.02	0.41
1:B:256:HIS:O	1:B:257:SER:CB	2.68	0.41
1:A:368:MET:HA	1:A:368:MET:HE3	2.02	0.41
1:B:201:THR:OG1	1:B:202:PRO:HD2	2.21	0.41
1:B:311:TYR:CE1	1:B:318:LYS:HD3	2.55	0.41
1:B:335:ASN:O	1:B:339:GLU:HG3	2.20	0.41
1:A:42:VAL:HA	1:A:68:LEU:HD21	2.01	0.41
1:A:249:ILE:O	1:A:306:PHE:HA	2.21	0.41
1:B:165:HIS:O	1:B:166:ASN:HB2	2.20	0.41
1:B:51:ARG:NH1	1:B:76:GLU:OE2	2.53	0.41
1:B:235:ARG:CD	1:B:240:ALA:O	2.69	0.41
1:A:68:LEU:O	1:A:73:SER:HB3	2.21	0.41
1:B:231:TYR:CE1	1:B:321:MET:HE3	2.56	0.41
1:A:34:ALA:HB3	1:A:41:MET:HE2	2.03	0.41
1:A:113:ILE:CG1	1:A:119:ILE:HD13	2.51	0.41
1:A:201:THR:OG1	1:A:204:GLN:HG3	2.21	0.41
1:A:339:GLU:HG2	5:A:3125:HOH:O	2.20	0.41
1:A:383:ASN:O	1:A:387:VAL:HG23	2.21	0.41
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.85	0.41
1:B:255:ILE:N	1:B:255:ILE:HD12	2.35	0.40
1:B:90:LEU:HB2	1:B:93:VAL:HG13	2.03	0.40
1:A:92:ASP:OD1	1:A:92:ASP:N	2.52	0.40
1:A:102:GLY:O	1:A:125:GLU:HG3	2.20	0.40
1:A:113:ILE:HA	1:A:119:ILE:HD11	2.04	0.40
1:A:216:LYS:HE3	5:A:3125:HOH:O	2.21	0.40
1:B:113:ILE:HD13	1:B:119:ILE:HG13	2.04	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	398/424 (94%)	385 (97%)	9 (2%)	4 (1%)	12	11
1	B	396/424 (93%)	384 (97%)	9 (2%)	3 (1%)	16	16
All	All	794/848 (94%)	769 (97%)	18 (2%)	7 (1%)	14	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	B	210	ASN
1	A	257	SER
1	B	257	SER
1	A	37	ASN
1	A	209	PRO
1	B	366	MET

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	328/347 (94%)	311 (95%)	17 (5%)	21	26
1	B	327/347 (94%)	311 (95%)	16 (5%)	22	29
All	All	655/694 (94%)	622 (95%)	33 (5%)	22	28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	LEU
1	A	16	THR
1	A	17	LEU
1	A	54	VAL
1	A	69	GLN
1	A	96	VAL
1	A	106	LEU
1	A	120	LEU
1	A	159	LEU
1	A	267	LEU
1	A	289	VAL
1	A	301	LEU
1	A	334	LEU
1	A	358	LEU
1	A	363	LEU
1	A	368	MET
1	B	3	LEU
1	B	6	LEU
1	B	20	VAL
1	B	41	MET
1	B	46	LEU
1	B	56	ASP
1	B	106	LEU
1	B	110	LEU
1	B	159	LEU
1	B	169	TYR
1	B	195	ARG
1	B	213	MET
1	B	235	ARG
1	B	269	GLN
1	B	301	LEU
1	B	334	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	26	HIS
1	A	44	GLN
1	A	71	GLN
1	A	123	ASN
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	164	GLN
1	A	165	HIS
1	A	175	ASN
1	A	208	HIS
1	A	226	ASN
1	A	239	ASN
1	A	244	GLN
1	A	252	GLN
1	A	256	HIS
1	A	281	HIS
1	A	328	GLN
1	A	349	GLN
1	A	383	ASN
1	B	2	GLN
1	B	26	HIS
1	B	69	GLN
1	B	70	GLN
1	B	71	GLN
1	B	82	GLN
1	B	140	GLN
1	B	144	GLN
1	B	152	HIS
1	B	157	GLN
1	B	161	GLN
1	B	164	GLN
1	B	166	ASN
1	B	175	ASN
1	B	244	GLN
1	B	252	GLN
1	B	256	HIS
1	B	269	GLN
1	B	281	HIS
1	B	290	ASN
1	B	349	GLN
1	B	372	GLN
1	B	383	ASN

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	FOM	A	1001	2	10,10,10	3.04	3 (30%)	11,13,13	2.37	4 (36%)
3	FOM	B	2001	2	10,10,10	3.16	2 (20%)	11,13,13	1.98	4 (36%)
4	NDP	A	3001	-	51,52,52	2.70	18 (35%)	71,80,80	3.58	35 (49%)
4	NDP	B	3002	-	51,52,52	2.75	21 (41%)	71,80,80	3.56	34 (47%)

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
3	FOM	A	1001	2	-	2/7/9/9	-
3	FOM	B	2001	2	-	2/7/9/9	-
4	NDP	A	3001	-	-	11/34/77/77	0/5/5/5
4	NDP	B	3002	-	-	11/34/77/77	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3002	NDP	PN-O3	8.19	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	FOM	O2-N1	-7.92	1.30	1.39
4	A	3001	NDP	PN-O3	7.45	1.67	1.59
4	A	3001	NDP	PN-O2N	-7.34	1.21	1.55
3	A	1001	FOM	O2-N1	-7.33	1.31	1.39
4	B	3002	NDP	PN-O2N	-7.33	1.21	1.55
4	B	3002	NDP	C4N-C3N	6.33	1.62	1.50
4	A	3001	NDP	C4N-C3N	5.99	1.61	1.50
4	A	3001	NDP	PA-O1A	-5.73	1.30	1.50
3	B	2001	FOM	PA1-OP1	5.36	1.61	1.50
4	B	3002	NDP	PA-O1A	-5.15	1.33	1.50
4	A	3001	NDP	C3B-C2B	5.12	1.64	1.53
3	A	1001	FOM	PA1-OP1	4.90	1.60	1.50
4	B	3002	NDP	C3B-C2B	4.86	1.63	1.53
4	B	3002	NDP	O5B-C5B	4.43	1.61	1.44
4	A	3001	NDP	O5B-C5B	4.42	1.61	1.44
4	A	3001	NDP	C2D-C3D	3.98	1.64	1.53
4	B	3002	NDP	C2D-C3D	3.96	1.64	1.53
4	A	3001	NDP	O3B-C3B	3.95	1.52	1.43
4	B	3002	NDP	O3B-C3B	3.76	1.52	1.43
4	B	3002	NDP	P2B-O2X	-3.33	1.42	1.54
4	A	3001	NDP	O4D-C1D	3.14	1.49	1.42
4	B	3002	NDP	PN-O1N	-3.14	1.39	1.50
4	B	3002	NDP	O4D-C1D	3.09	1.49	1.42
4	B	3002	NDP	PA-O3	-3.02	1.56	1.59
4	A	3001	NDP	C7N-C3N	2.92	1.55	1.48
4	A	3001	NDP	P2B-O2X	-2.91	1.44	1.54
4	A	3001	NDP	PN-O1N	-2.62	1.41	1.50
4	A	3001	NDP	C4N-C5N	2.60	1.55	1.49
4	B	3002	NDP	C7N-C3N	2.59	1.54	1.48
4	B	3002	NDP	C4N-C5N	2.58	1.55	1.49
4	B	3002	NDP	O4B-C1B	2.58	1.48	1.42
4	B	3002	NDP	P2B-O2B	-2.57	1.55	1.59
4	A	3001	NDP	PA-O3	-2.54	1.56	1.59
4	A	3001	NDP	O5D-C5D	-2.44	1.35	1.44
4	B	3002	NDP	O5D-C5D	-2.39	1.35	1.44
4	B	3002	NDP	C8A-N9A	2.34	1.41	1.37
3	A	1001	FOM	PA1-OP2	2.31	1.60	1.55
4	B	3002	NDP	C6A-N1A	2.26	1.42	1.35
4	A	3001	NDP	C3D-C4D	-2.19	1.47	1.53
4	B	3002	NDP	C1D-N1N	2.10	1.52	1.46
4	B	3002	NDP	C7N-N7N	2.08	1.39	1.33
4	A	3001	NDP	C6A-N1A	2.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	NDP	C1D-N1N	2.05	1.52	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	NDP	O2A-PA-O3	-11.17	77.09	107.27
4	B	3002	NDP	O2A-PA-O3	-10.61	78.60	107.27
4	B	3002	NDP	O2B-C2B-C3B	-10.08	75.53	111.68
4	A	3001	NDP	O2B-C2B-C3B	-9.97	75.91	111.68
4	A	3001	NDP	C2D-C3D-C4D	-8.37	86.44	102.61
4	B	3002	NDP	O4D-C4D-C3D	7.58	120.20	105.15
4	B	3002	NDP	C2D-C3D-C4D	-6.97	89.14	102.61
4	A	3001	NDP	O3-PA-O1A	-6.88	90.00	110.70
4	B	3002	NDP	O3-PA-O1A	-6.66	90.66	110.70
4	B	3002	NDP	O2N-PN-O5D	-6.54	77.91	107.57
4	A	3001	NDP	O2N-PN-O5D	-6.40	78.54	107.57
4	A	3001	NDP	O4D-C4D-C3D	6.37	117.79	105.15
4	B	3002	NDP	O4D-C1D-N1N	-5.47	97.66	108.08
4	A	3001	NDP	N9A-C8A-N7A	-5.43	106.23	113.94
4	B	3002	NDP	N9A-C8A-N7A	-5.19	106.57	113.94
4	A	3001	NDP	O4D-C1D-N1N	-5.15	98.27	108.08
4	A	3001	NDP	C4A-N9A-C1B	-5.11	114.69	126.63
4	A	3001	NDP	P2B-O2B-C2B	-5.08	109.88	123.43
4	A	3001	NDP	O4D-C4D-C5D	5.05	125.51	109.33
4	B	3002	NDP	P2B-O2B-C2B	-5.00	110.08	123.43
4	B	3002	NDP	C4A-N9A-C1B	-4.94	115.07	126.63
4	B	3002	NDP	O4D-C4D-C5D	4.84	124.84	109.33
4	B	3002	NDP	O3B-C3B-C4B	-4.54	98.05	111.08
4	A	3001	NDP	C4A-N9A-C8A	4.52	110.49	105.74
4	B	3002	NDP	O2N-PN-O3	-4.51	95.09	107.27
4	A	3001	NDP	O2N-PN-O3	-4.40	95.39	107.27
4	A	3001	NDP	O4B-C1B-C2B	4.36	114.10	106.59
4	B	3002	NDP	C2D-C1D-N1N	4.32	123.92	113.31
4	B	3002	NDP	O4B-C4B-C5B	4.29	123.09	109.33
4	A	3001	NDP	O4B-C4B-C5B	4.27	123.01	109.33
3	A	1001	FOM	OP3-PA1-C4	4.20	116.95	106.91
4	B	3002	NDP	O2B-C2B-C1B	4.16	124.67	110.05
4	B	3002	NDP	C3B-C2B-C1B	-4.11	94.94	102.81
4	B	3002	NDP	C4A-N9A-C8A	4.11	110.05	105.74
3	B	2001	FOM	OP3-PA1-C4	4.09	116.67	106.91
4	A	3001	NDP	C4D-O4D-C1D	-4.09	100.45	109.47
4	A	3001	NDP	O2B-C2B-C1B	4.08	124.39	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	NDP	C2D-C1D-N1N	4.07	123.33	113.31
4	A	3001	NDP	C3B-C2B-C1B	-4.02	95.11	102.81
4	A	3001	NDP	C2B-C1B-N9A	-4.02	107.14	113.75
4	B	3002	NDP	C4D-O4D-C1D	-4.01	100.60	109.47
3	A	1001	FOM	PA1-C4-C3	4.00	119.87	114.94
4	A	3001	NDP	O3B-C3B-C4B	-4.00	99.60	111.08
4	B	3002	NDP	C2B-C1B-N9A	-3.98	107.20	113.75
4	B	3002	NDP	O4B-C1B-C2B	3.91	113.31	106.59
4	B	3002	NDP	C2B-C3B-C4B	3.89	110.35	101.99
4	A	3001	NDP	O2A-PA-O1A	3.88	130.48	112.44
4	B	3002	NDP	O4B-C1B-N9A	-3.83	100.74	108.09
4	B	3002	NDP	O2A-PA-O1A	3.82	130.21	112.44
4	A	3001	NDP	C2B-C3B-C4B	3.81	110.19	101.99
4	A	3001	NDP	C5A-N7A-C8A	3.66	109.21	103.45
4	B	3002	NDP	C5A-N7A-C8A	3.57	109.07	103.45
4	B	3002	NDP	C1B-N9A-C8A	3.46	134.78	127.09
4	A	3001	NDP	C1B-N9A-C8A	3.45	134.75	127.09
4	A	3001	NDP	O5D-PN-O1N	3.44	122.58	108.94
4	B	3002	NDP	O5D-PN-O1N	3.40	122.42	108.94
4	B	3002	NDP	O3D-C3D-C2D	3.33	122.50	111.82
4	A	3001	NDP	O3D-C3D-C2D	3.32	122.44	111.82
4	A	3001	NDP	O4B-C1B-N9A	-3.31	101.73	108.09
4	B	3002	NDP	O3D-C3D-C4D	-3.03	102.37	111.08
3	B	2001	FOM	OP2-PA1-OP1	-3.00	104.62	112.39
4	A	3001	NDP	C6A-C5A-N7A	2.94	137.76	132.09
4	B	3002	NDP	C6A-C5A-N7A	2.93	137.73	132.09
3	A	1001	FOM	OP2-PA1-OP1	-2.86	104.99	112.39
4	A	3001	NDP	O2N-PN-O1N	-2.75	99.66	112.44
4	A	3001	NDP	C6A-C5A-C4A	-2.56	113.68	117.18
4	B	3002	NDP	O2N-PN-O1N	-2.56	100.54	112.44
4	B	3002	NDP	C6A-C5A-C4A	-2.55	113.69	117.18
4	B	3002	NDP	O5D-C5D-C4D	-2.52	100.42	108.99
4	B	3002	NDP	C5D-C4D-C3D	-2.45	106.40	115.21
4	A	3001	NDP	O5D-C5D-C4D	-2.43	100.73	108.99
4	A	3001	NDP	O3D-C3D-C4D	-2.21	104.75	111.08
3	A	1001	FOM	O1-C1-N1	2.20	131.11	125.49
4	A	3001	NDP	N3A-C2A-N1A	-2.18	125.29	128.58
3	B	2001	FOM	O1-C1-N1	2.15	130.99	125.49
3	B	2001	FOM	O2-N1-C2	2.07	118.61	113.81
4	A	3001	NDP	O3X-P2B-O2X	2.01	115.34	107.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FOM	N1-C2-C3-C4
3	A	1001	FOM	C2-C3-C4-PA1
4	A	3001	NDP	C5B-O5B-PA-O1A
4	A	3001	NDP	C5B-O5B-PA-O3
4	A	3001	NDP	C5D-O5D-PN-O2N
4	A	3001	NDP	O4D-C4D-C5D-O5D
4	B	3002	NDP	C5B-O5B-PA-O3
4	B	3002	NDP	C5D-O5D-PN-O2N
4	B	3002	NDP	O4D-C4D-C5D-O5D
4	B	3002	NDP	C3D-C4D-C5D-O5D
4	B	3002	NDP	O4D-C1D-N1N-C6N
4	A	3001	NDP	O4D-C1D-N1N-C6N
4	A	3001	NDP	C5D-O5D-PN-O3
4	B	3002	NDP	C5D-O5D-PN-O3
4	B	3002	NDP	O4B-C4B-C5B-O5B
4	A	3001	NDP	O4B-C4B-C5B-O5B
4	A	3001	NDP	C2N-C3N-C7N-N7N
4	B	3002	NDP	C2N-C3N-C7N-N7N
4	A	3001	NDP	C2B-O2B-P2B-O1X
4	B	3002	NDP	C2B-O2B-P2B-O1X
3	B	2001	FOM	N1-C2-C3-C4
4	A	3001	NDP	C3D-C4D-C5D-O5D
3	B	2001	FOM	C3-C2-N1-O2
4	A	3001	NDP	PA-O3-PN-O2N
4	B	3002	NDP	PN-O3-PA-O2A
4	B	3002	NDP	PA-O3-PN-O2N

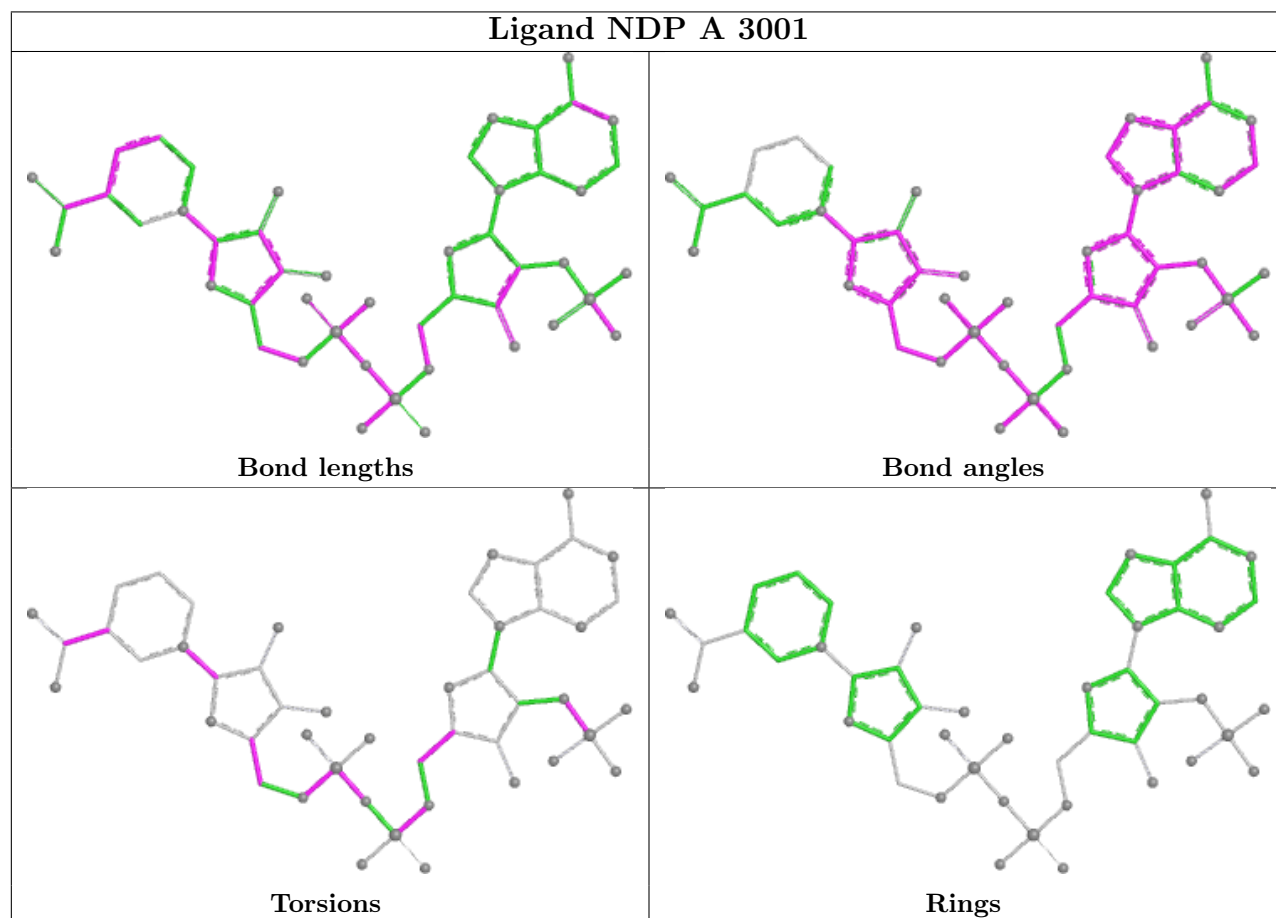
There are no ring outliers.

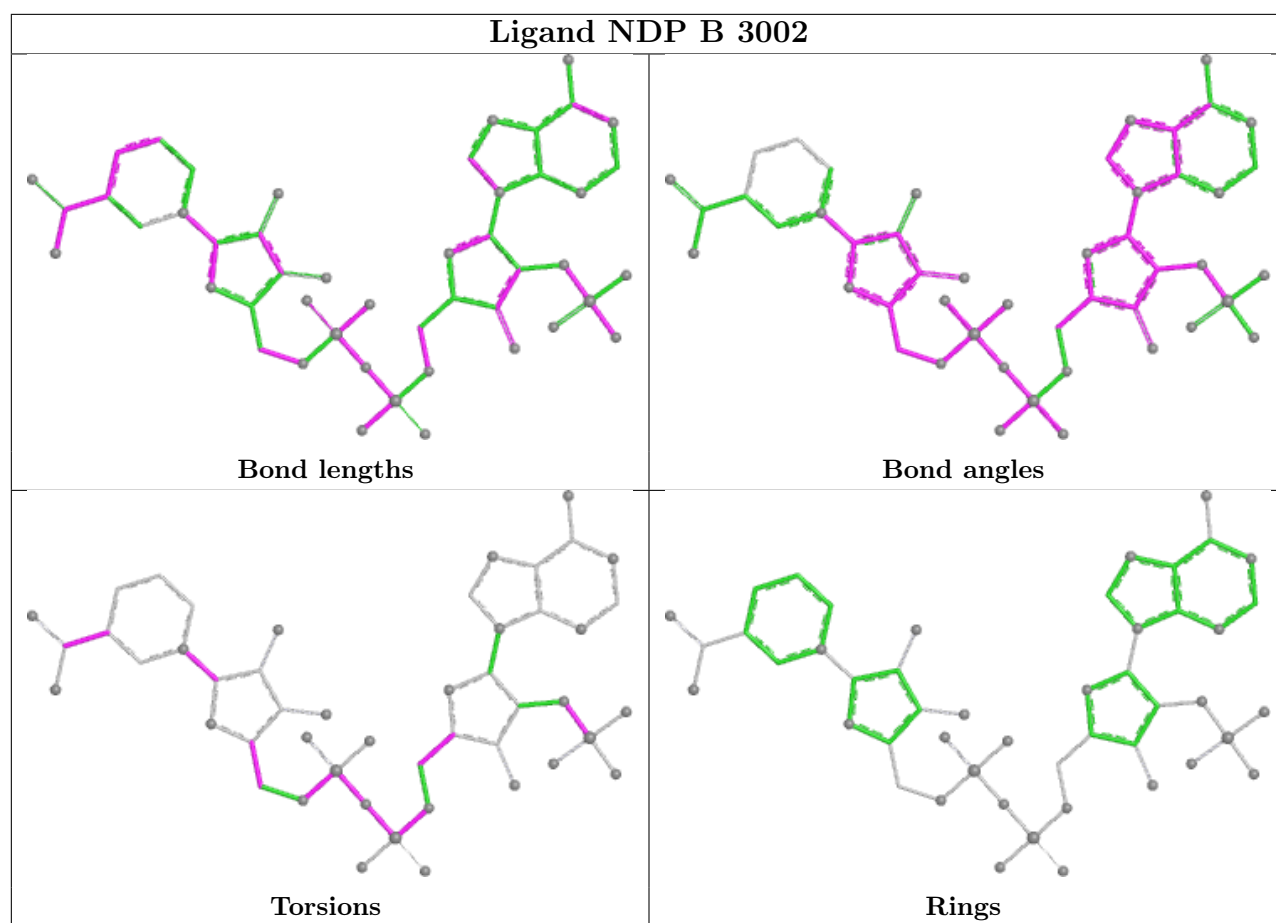
2 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	NDP	10	0
4	B	3002	NDP	18	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	400/424 (94%)	0.38	35 (8%) 15 13	22, 34, 72, 98	0
1	B	398/424 (93%)	0.31	24 (6%) 27 24	23, 37, 60, 86	0
All	All	798/848 (94%)	0.34	59 (7%) 20 18	22, 35, 66, 98	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	ALA	6.9
1	A	211	TRP	5.1
1	A	0	GLY	4.9
1	A	210	ASN	4.4
1	B	0	GLY	4.2
1	A	67	MET	4.1
1	B	169	TYR	4.1
1	A	368	MET	4.0
1	A	212	SER	4.0
1	A	398	SER	4.0
1	A	209	PRO	3.8
1	A	208	HIS	3.7
1	A	63	LEU	3.5
1	A	395	LEU	3.5
1	A	169	TYR	3.3
1	A	70	GLN	3.2
1	B	369	ARG	3.1
1	A	66	THR	3.1
1	B	126	SER	3.1
1	B	210	ASN	3.1
1	A	3	LEU	3.1
1	A	213	MET	3.0
1	B	209	PRO	3.0
1	A	68	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	367	ASP	2.9
1	B	211	TRP	2.8
1	B	397	SER	2.7
1	A	396	ALA	2.7
1	A	65	LYS	2.6
1	B	368	MET	2.6
1	A	69	GLN	2.6
1	A	92	ASP	2.6
1	B	383	ASN	2.6
1	B	366	MET	2.5
1	A	26	HIS	2.5
1	B	66	THR	2.5
1	A	367	ASP	2.5
1	A	73	SER	2.3
1	A	72	GLY	2.3
1	B	67	MET	2.3
1	A	43	GLU	2.3
1	A	48	PHE	2.3
1	B	142	LYS	2.3
1	B	394	ARG	2.2
1	A	61	ALA	2.2
1	A	62	LYS	2.2
1	A	64	LEU	2.2
1	B	3	LEU	2.2
1	B	370	GLU	2.2
1	A	369	ARG	2.1
1	A	46	LEU	2.1
1	B	217	ILE	2.1
1	B	208	HIS	2.1
1	B	132	ARG	2.1
1	B	91	GLU	2.0
1	A	394	ARG	2.0
1	A	58	GLU	2.0
1	B	143	ALA	2.0
1	B	207	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

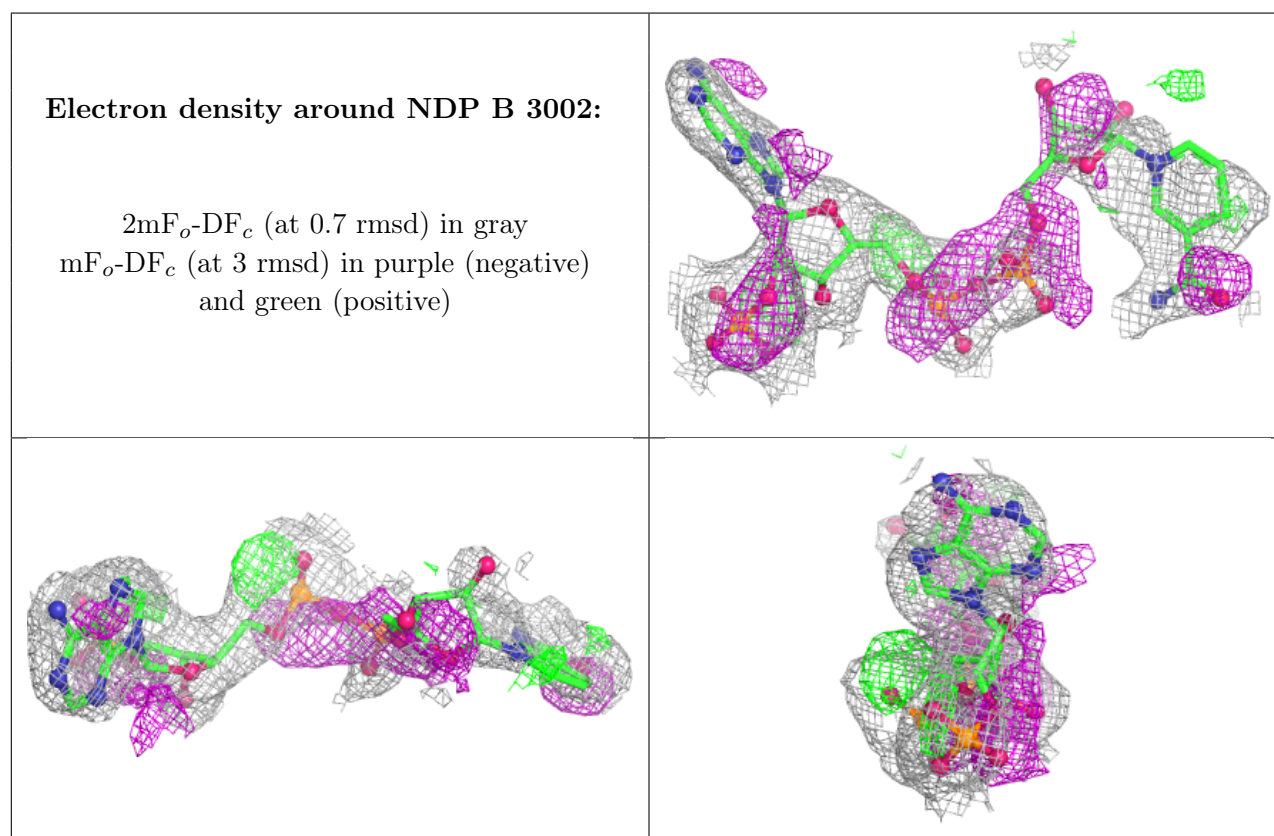
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

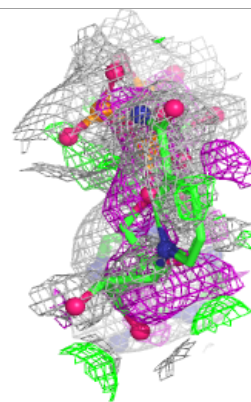
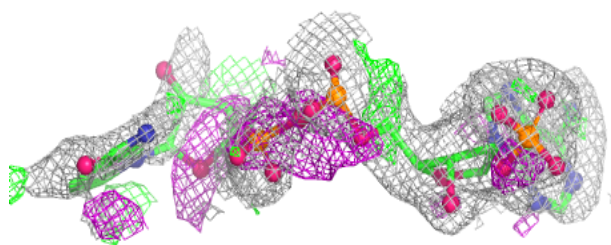
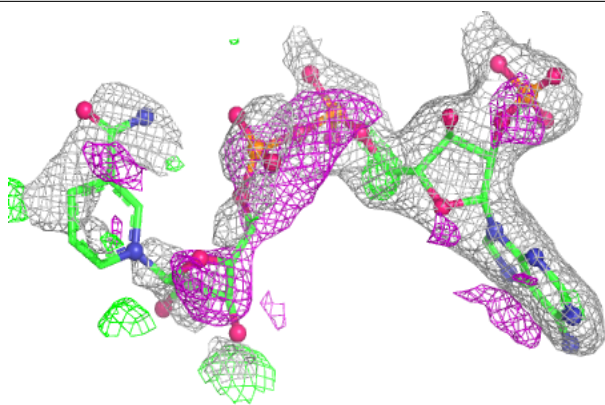
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NDP	B	3002	48/48	0.67	0.23	56,78,85,85	0
4	NDP	A	3001	48/48	0.69	0.23	59,81,91,91	0
3	FOM	A	1001	11/11	0.78	0.20	75,77,77,78	0
3	FOM	B	2001	11/11	0.81	0.20	73,74,75,75	0
2	MG	A	900	1/1	0.91	0.07	65,65,65,65	0
2	MG	B	901	1/1	0.97	0.05	53,53,53,53	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 A 3001:

$2mF_o-DF_c$ (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.