



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 06:55 PM UTC

PDB ID : 1RM5 / pdb_00001rm5
Title : Crystal structure of mutant S188A of photosynthetic glyceraldehyde-3-phosphate dehydrogenase A4 isoform, complexed with NADP
Authors : Sparla, F.; Fermani, S.; Falini, G.; Ripamonti, A.; Sabatino, P.; Pupillo, P.; Trost, P.
Deposited on : 2003-11-27
Resolution : 2.10 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

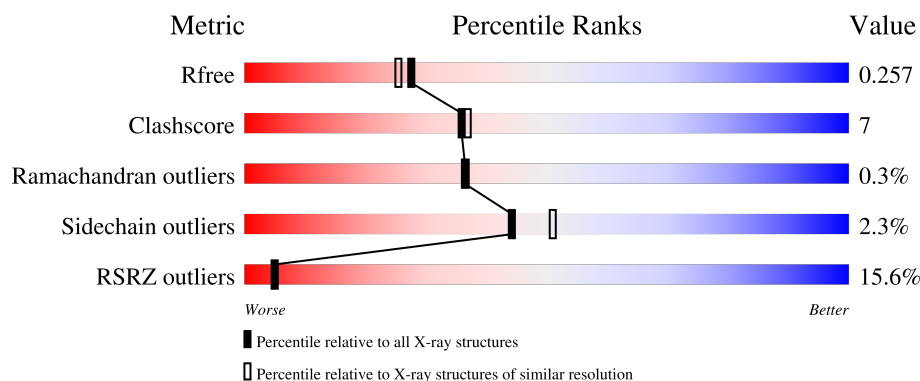
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	337	16% 82% 16%
1	B	337	28% 85% 13%
1	O	337	2% 84% 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8363 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 Glyceraldehyde 3-phosphate dehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	337	Total	C	N	O	S	0	10	0
			2576	1620	447	495	14			
1	A	337	Total	C	N	O	S	0	4	0
			2557	1608	446	490	13			
1	B	337	Total	C	N	O	S	0	4	0
			2555	1607	445	490	13			

There are 3 discrepancies between the modelled and reference sequences:

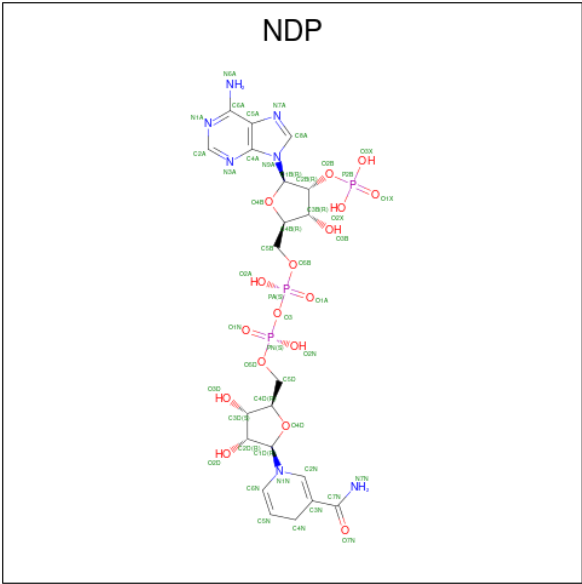
Chain	Residue	Modelled	Actual	Comment	Reference
O	188	ALA	SER	engineered mutation	UNP P19866
A	188	ALA	SER	engineered mutation	UNP P19866
B	188	ALA	SER	engineered mutation	UNP P19866

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



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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

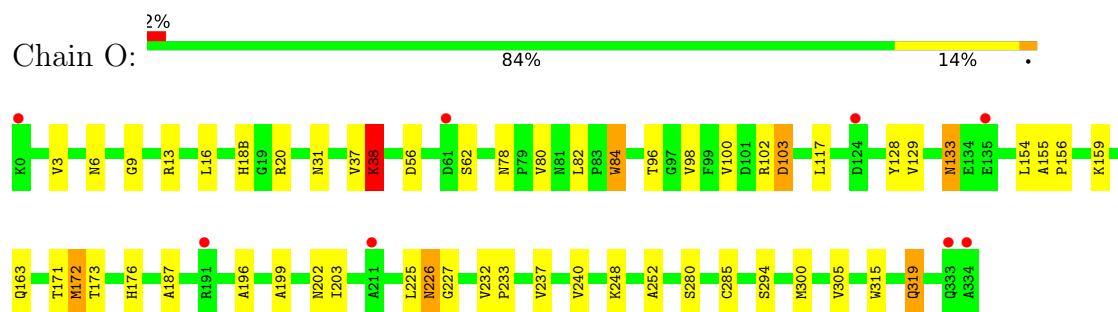
- Molecule 4 is water.

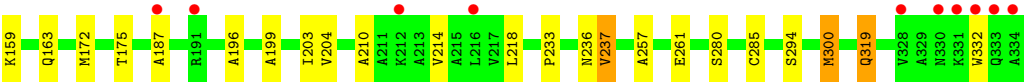
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	214	Total	O	0	0
			214	214		
4	A	134	Total	O	0	0
			134	134		
4	B	133	Total	O	0	0
			133	133		

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: Glyceraldehyde 3-phosphate dehydrogenase A





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	143.90Å 190.29Å 109.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.06 – 2.10 79.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (79.06-2.10) 97.9 (79.06-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.24 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.254 0.225 , 0.257	Depositor DCC
R_{free} test set	4336 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.7	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	8363	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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

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, SO4

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	0.49	0/2614	0.99	13/3548 (0.4%)
1	B	0.48	0/2612	0.97	15/3545 (0.4%)
1	O	0.68	0/2657	1.07	24/3604 (0.7%)
All	All	0.56	0/7883	1.01	52/10697 (0.5%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	VAL	N-CA-C	10.39	118.44	108.15
1	A	199	ALA	N-CA-C	9.82	122.07	111.36
1	A	204	VAL	N-CA-C	9.05	117.29	107.60
1	O	199	ALA	N-CA-C	8.46	120.50	111.28
1	O	62	SER	N-CA-C	8.02	119.88	110.41
1	O	203	ILE	N-CA-C	-7.75	96.67	107.99
1	B	199	ALA	N-CA-C	7.34	120.15	111.71
1	B	203	ILE	N-CA-C	-7.08	97.66	107.99
1	A	203	ILE	N-CA-C	-6.90	97.16	107.37
1	O	252	ALA	N-CA-C	6.85	119.33	111.11
1	O	38[A]	LYS	CB-CA-C	6.69	122.22	110.85
1	O	38[B]	LYS	CB-CA-C	6.69	122.22	110.85
1	O	280	SER	N-CA-C	6.54	119.24	111.33
1	B	294	SER	N-CA-C	6.54	119.24	111.33
1	A	300[A]	MET	CB-CA-C	-6.46	98.54	109.72
1	A	300[B]	MET	CB-CA-C	-6.46	98.54	109.72
1	B	280	SER	N-CA-C	6.24	118.88	111.33
1	O	154	LEU	N-CA-C	6.24	117.88	111.14
1	O	294	SER	N-CA-C	6.22	118.86	111.33
1	O	176	HIS	N-CA-C	6.19	119.56	109.59
1	O	3	VAL	N-CA-C	6.18	117.49	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	202	ASN	N-CA-C	6.00	118.29	109.24
1	A	202	ASN	N-CA-C	5.96	118.46	109.41
1	O	300[A]	MET	CB-CA-C	5.84	119.89	109.38
1	O	300[B]	MET	CB-CA-C	5.84	119.89	109.38
1	O	100	VAL	N-CA-C	5.80	118.57	112.83
1	B	218	LEU	CA-C-N	5.79	127.08	119.84
1	B	218	LEU	C-N-CA	5.79	127.08	119.84
1	B	300[A]	MET	N-CA-CB	5.77	119.63	110.57
1	B	300[B]	MET	N-CA-CB	5.77	119.63	110.57
1	A	3	VAL	N-CA-C	5.72	116.82	108.53
1	O	103[A]	ASP	CB-CA-C	5.56	120.02	110.79
1	O	103[B]	ASP	CB-CA-C	5.56	120.02	110.79
1	O	315	TRP	N-CA-C	5.55	117.14	111.14
1	O	233	PRO	N-CA-C	5.48	123.76	112.47
1	O	102	ARG	N-CA-C	5.44	116.89	111.07
1	B	78	ASN	CA-C-N	5.42	125.50	119.32
1	B	78	ASN	C-N-CA	5.42	125.50	119.32
1	A	56[A]	ASP	N-CA-CB	-5.40	101.30	109.94
1	A	56[B]	ASP	N-CA-CB	-5.40	101.30	109.94
1	B	56[A]	ASP	CB-CA-C	5.34	119.69	110.77
1	B	56[B]	ASP	CB-CA-C	5.34	119.69	110.77
1	A	235	PRO	N-CA-C	5.29	120.50	113.57
1	B	233	PRO	N-CA-C	5.29	123.36	112.47
1	A	112	GLY	N-CA-C	5.27	120.75	114.48
1	O	305	VAL	N-CA-C	5.26	115.88	108.36
1	O	56[A]	ASP	N-CA-CB	-5.21	101.60	109.94
1	O	56[B]	ASP	N-CA-CB	-5.21	101.60	109.94
1	A	315	TRP	N-CA-C	5.16	116.72	111.14
1	O	232	VAL	N-CA-C	5.14	113.55	107.84
1	A	265	ASN	N-CA-C	5.08	116.22	108.30
1	B	175	THR	N-CA-C	-5.04	100.30	108.41

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	2557	0	2586	51	0
1	B	2555	0	2585	29	0
1	O	2576	0	2605	36	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
2	O	15	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	1	0
3	O	48	0	26	0	0
4	A	134	0	0	2	0
4	B	133	0	0	0	0
4	O	214	0	0	2	0
All	All	8363	0	7854	115	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 (115) 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:O:6:ASN:HD21	1:O:31:ASN:HD22	1.26	0.82
1:O:37:VAL:HG13	1:O:38[B]:LYS:HD2	1.62	0.78
1:A:78:ASN:ND2	1:A:80:VAL:HG12	2.00	0.77
1:O:6:ASN:ND2	1:O:31:ASN:HD22	1.83	0.76
1:A:170:GLY:HA3	1:A:244:VAL:HG12	1.68	0.76
1:O:78:ASN:OD1	1:O:80:VAL:HG22	1.88	0.73
1:A:6:ASN:ND2	1:A:31:ASN:HD22	1.88	0.72
1:O:172[A]:MET:HG2	1:O:173:THR:N	2.05	0.72
1:A:171:THR:HA	1:A:226[B]:ASN:ND2	2.04	0.72
1:A:6:ASN:HD21	1:A:31:ASN:HD22	1.36	0.71
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.71	0.71
1:B:78:ASN:OD1	1:B:80:VAL:HG22	1.91	0.70
1:A:224:LYS:C	1:A:225:LEU:HD12	2.18	0.68
1:O:20:ARG:HH21	1:O:319:GLN:NE2	1.92	0.66
1:A:171:THR:CB	1:A:226[B]:ASN:HD21	2.09	0.66
1:A:20:ARG:HH21	1:A:319:GLN:NE2	1.95	0.64
1:B:20:ARG:HH11	1:B:319:GLN:HE22	1.46	0.63
1:B:319:GLN:HE21	1:B:319:GLN:HA	1.64	0.63
1:A:171:THR:HA	1:A:226[B]:ASN:HD21	1.65	0.61
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.36	0.61
1:B:129:VAL:H	1:B:133:ASN:HD21	1.48	0.60
1:O:172[A]:MET:HG2	1:O:173:THR:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:37:VAL:HG13	1:O:38[B]:LYS:CD	2.32	0.59
1:A:0:LYS:HB3	1:A:0:LYS:NZ	2.18	0.59
1:O:319:GLN:HE21	1:O:319:GLN:HA	1.68	0.58
1:O:159:LYS:O	1:O:163:GLN:HG3	2.04	0.58
1:A:171:THR:CA	1:A:226[B]:ASN:HD21	2.17	0.57
1:B:20:ARG:HH11	1:B:319:GLN:NE2	2.01	0.57
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.86	0.57
1:A:78:ASN:HD21	1:A:80:VAL:HG12	1.70	0.56
1:A:158:VAL:CG1	1:A:221:LEU:HD21	2.36	0.56
1:O:96:THR:OG1	1:O:98:VAL:HG22	2.05	0.56
1:O:172[A]:MET:HG3	1:O:240:VAL:HG13	1.87	0.56
1:B:210:ALA:O	1:B:214:VAL:HG23	2.06	0.56
1:A:190:HIS:H	1:B:39:GLN:NE2	2.04	0.55
1:A:319:GLN:HA	1:A:319:GLN:HE21	1.72	0.55
1:B:90:ASP:HA	1:B:114:LYS:HD2	1.89	0.55
1:O:18(B):HIS:HD2	4:O:7519:HOH:O	1.89	0.54
1:B:129:VAL:H	1:B:133:ASN:ND2	2.05	0.53
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.44	0.53
1:A:154:LEU:HD11	1:A:172:MET:HE3	1.91	0.53
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.09	0.53
1:B:74:VAL:HG12	1:B:75:SER:N	2.25	0.52
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.92	0.51
1:A:34:GLY:HA3	1:A:39:GLN:OE1	2.12	0.50
1:O:20:ARG:HH21	1:O:319:GLN:HE21	1.60	0.50
1:B:84:TRP:HE3	1:B:84:TRP:HA	1.77	0.49
1:O:129:VAL:H	1:O:133:ASN:HD21	1.59	0.49
1:A:236:ASN:O	1:A:237:VAL:HB	2.11	0.49
1:B:20:ARG:NH1	1:B:319:GLN:NE2	2.60	0.49
1:B:84:TRP:HA	1:B:84:TRP:CE3	2.47	0.49
1:A:20:ARG:HH21	1:A:319:GLN:HE21	1.59	0.48
1:A:0:LYS:HB3	1:A:0:LYS:HZ3	1.78	0.48
1:B:11:ILE:HD11	3:B:2335:NDP:H42N	1.96	0.47
1:A:226[A]:ASN:ND2	1:A:227:GLY:H	2.13	0.47
1:A:78:ASN:HD22	1:A:78:ASN:C	2.22	0.47
1:O:129:VAL:H	1:O:133:ASN:ND2	2.12	0.47
1:A:279:VAL:HG22	1:A:280:SER:N	2.30	0.47
1:A:221:LEU:HD12	1:A:221:LEU:N	2.30	0.46
1:O:171:THR:CB	1:O:226[A]:ASN:HD21	2.28	0.46
1:O:20:ARG:HE	1:O:319:GLN:HE22	1.64	0.46
1:A:117:LEU:C	1:A:117:LEU:HD23	2.40	0.46
1:B:187:ALA:O	1:B:196:ALA:HB1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.81	0.46
1:A:129:VAL:H	1:A:133:ASN:HD21	1.62	0.46
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.97	0.45
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.52	0.45
1:A:129:VAL:H	1:A:133:ASN:ND2	2.14	0.45
1:O:226[B]:ASN:ND2	1:O:227:GLY:H	2.14	0.45
1:B:236:ASN:O	1:B:237:VAL:HB	2.17	0.45
1:A:9:GLY:O	1:A:13:ARG:HG3	2.17	0.44
1:A:187:ALA:O	1:A:196:ALA:HB1	2.18	0.44
1:A:300[A]:MET:HE3	1:A:300[A]:MET:HB2	1.87	0.44
1:A:225:LEU:HD12	1:A:225:LEU:N	2.33	0.44
1:A:250:THR:OG1	1:A:251:PHE:N	2.51	0.44
1:O:226[B]:ASN:HD22	1:O:227:GLY:H	1.65	0.43
1:O:117:LEU:C	1:O:117:LEU:HD23	2.43	0.43
1:B:85:GLY:CA	1:B:112:GLY:HA3	2.48	0.43
1:A:78:ASN:CG	1:A:80:VAL:HG12	2.43	0.43
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.83	0.43
1:B:132:VAL:HG21	1:B:155:ALA:HB1	2.01	0.43
1:O:248:LYS:HE3	4:O:7485:HOH:O	2.19	0.43
1:O:9:GLY:O	1:O:13:ARG:HG3	2.19	0.43
1:O:171:THR:HA	1:O:226[A]:ASN:ND2	2.34	0.43
1:A:171:THR:HB	1:A:226[B]:ASN:HD21	1.81	0.42
1:A:72:LYS:HG3	1:A:73:VAL:N	2.33	0.42
1:B:32:ASP:C	1:B:34:GLY:H	2.28	0.42
1:B:90:ASP:O	1:B:114:LYS:HB2	2.20	0.42
1:B:154:LEU:HD11	1:B:172:MET:SD	2.60	0.41
1:A:158:VAL:HG12	1:A:221:LEU:HD21	2.02	0.41
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.42	0.41
1:B:9:GLY:O	1:B:13:ARG:HG3	2.20	0.41
1:A:103:ASP:HB2	4:A:1420:HOH:O	2.19	0.41
1:O:172[A]:MET:HE2	1:O:172[A]:MET:HB3	1.74	0.41
1:A:221:LEU:N	1:A:221:LEU:CD1	2.84	0.41
1:A:292:ILE:HD13	1:A:309:ALA:HB2	2.02	0.41
1:A:77:ARG:HG2	4:A:1426:HOH:O	2.21	0.41
1:A:133:ASN:ND2	1:A:133:ASN:C	2.77	0.41
1:A:251:PHE:N	1:A:251:PHE:CD1	2.89	0.41
1:B:133:ASN:ND2	1:B:133:ASN:C	2.79	0.41
1:B:159:LYS:O	1:B:163:GLN:HG3	2.21	0.41
1:A:279:VAL:HG22	1:A:280:SER:H	1.86	0.40
1:O:187:ALA:O	1:O:196:ALA:HB1	2.21	0.40
1:O:16:LEU:HD13	1:O:16:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:O	1:B:261:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/337 (101%)	316 (93%)	22 (6%)	1 (0%)	36	36
1	B	339/337 (101%)	316 (93%)	22 (6%)	1 (0%)	36	36
1	O	345/337 (102%)	328 (95%)	16 (5%)	1 (0%)	36	36
All	All	1023/1011 (101%)	960 (94%)	60 (6%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	237	VAL
1	A	237	VAL
1	B	237	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/278 (101%)	275 (98%)	7 (2%)	42	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	282/278 (101%)	277 (98%)	5 (2%)	51	60
1	O	288/278 (104%)	275 (96%)	13 (4%)	24	25
All	All	852/834 (102%)	827 (97%)	25 (3%)	44	42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	38[A]	LYS
1	O	38[B]	LYS
1	O	84	TRP
1	O	103[A]	ASP
1	O	103[B]	ASP
1	O	133	ASN
1	O	172[A]	MET
1	O	172[B]	MET
1	O	225	LEU
1	O	226[A]	ASN
1	O	226[B]	ASN
1	O	285	CYS
1	O	319	GLN
1	A	84	TRP
1	A	133	ASN
1	A	226[A]	ASN
1	A	226[B]	ASN
1	A	300[A]	MET
1	A	300[B]	MET
1	A	319	GLN
1	B	84	TRP
1	B	133	ASN
1	B	285	CYS
1	B	319	GLN
1	B	332	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	6	ASN
1	O	18(B)	HIS
1	O	81	ASN
1	O	133	ASN

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Mol	Chain	Res	Type
1	O	236	ASN
1	O	256	ASN
1	O	319	GLN
1	A	6	ASN
1	A	78	ASN
1	A	81	ASN
1	A	133	ASN
1	A	152	ASN
1	A	236	ASN
1	A	256	ASN
1	A	319	GLN
1	A	330	ASN
1	A	333	GLN
1	B	6	ASN
1	B	39	GLN
1	B	133	ASN
1	B	256	ASN
1	B	265	ASN
1	B	319	GLN
1	B	330	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](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NDP	O	7335	-	51,52,52	1.56	8 (15%)	71,80,80	2.20	22 (30%)
2	SO4	A	1338	-	4,4,4	0.36	0	6,6,6	0.06	0
2	SO4	O	7339	-	4,4,4	0.39	0	6,6,6	0.04	0
2	SO4	A	901	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	B	2338	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	B	2339	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	A	1339	-	4,4,4	0.37	0	6,6,6	0.05	0
2	SO4	B	904	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	O	902	-	4,4,4	0.40	0	6,6,6	0.13	0
2	SO4	A	903	-	4,4,4	0.37	0	6,6,6	0.09	0
3	NDP	A	1335	-	51,52,52	1.55	8 (15%)	71,80,80	2.18	21 (29%)
3	NDP	B	2335	-	51,52,52	1.56	8 (15%)	71,80,80	2.18	21 (29%)
2	SO4	O	7338	-	4,4,4	0.33	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	O	7335	-	-	8/34/77/77	0/5/5/5
3	NDP	A	1335	-	-	6/34/77/77	0/5/5/5
3	NDP	B	2335	-	-	5/34/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	7335	NDP	C4N-C3N	-5.71	1.39	1.50
3	B	2335	NDP	C4N-C3N	-5.70	1.39	1.50
3	A	1335	NDP	C4N-C3N	-5.70	1.39	1.50
3	O	7335	NDP	P2B-O1X	4.13	1.63	1.50
3	B	2335	NDP	P2B-O1X	4.13	1.63	1.50
3	A	1335	NDP	P2B-O1X	4.12	1.63	1.50
3	A	1335	NDP	C4N-C5N	-3.65	1.39	1.49
3	O	7335	NDP	C4N-C5N	-3.61	1.39	1.49
3	B	2335	NDP	C4N-C5N	-3.57	1.39	1.49
3	O	7335	NDP	C5A-N7A	-3.08	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2335	NDP	C5A-N7A	-3.05	1.33	1.39
3	O	7335	NDP	C7N-C3N	3.00	1.55	1.48
3	A	1335	NDP	C5A-N7A	-2.98	1.33	1.39
3	A	1335	NDP	C7N-C3N	2.95	1.55	1.48
3	B	2335	NDP	C7N-C3N	2.95	1.55	1.48
3	B	2335	NDP	C4A-N9A	-2.45	1.32	1.37
3	A	1335	NDP	C4A-N9A	-2.38	1.32	1.37
3	O	7335	NDP	C4A-N9A	-2.34	1.32	1.37
3	A	1335	NDP	C2N-C3N	2.30	1.41	1.35
3	A	1335	NDP	C6N-C5N	2.29	1.40	1.33
3	O	7335	NDP	C6N-C5N	2.29	1.40	1.33
3	B	2335	NDP	C6N-C5N	2.28	1.40	1.33
3	O	7335	NDP	C2N-C3N	2.26	1.41	1.35
3	B	2335	NDP	C2N-C3N	2.25	1.41	1.35

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	7335	NDP	N3A-C4A-N9A	7.41	139.78	127.17
3	B	2335	NDP	N3A-C4A-N9A	7.37	139.71	127.17
3	A	1335	NDP	N3A-C4A-N9A	7.34	139.65	127.17
3	O	7335	NDP	C5A-C4A-N3A	-6.02	118.43	126.72
3	B	2335	NDP	C5A-C4A-N3A	-6.00	118.46	126.72
3	A	1335	NDP	C5A-C4A-N3A	-5.99	118.47	126.72
3	B	2335	NDP	C4A-N9A-C8A	5.09	111.08	105.74
3	O	7335	NDP	C4A-N9A-C8A	5.04	111.03	105.74
3	A	1335	NDP	C4A-N9A-C8A	4.97	110.96	105.74
3	O	7335	NDP	N3A-C2A-N1A	-4.23	122.17	128.58
3	A	1335	NDP	N3A-C2A-N1A	-4.21	122.21	128.58
3	O	7335	NDP	C4B-O4B-C1B	-4.19	100.20	109.47
3	A	1335	NDP	C4B-O4B-C1B	-4.17	100.25	109.47
3	B	2335	NDP	C4B-O4B-C1B	-4.15	100.30	109.47
3	B	2335	NDP	N3A-C2A-N1A	-4.13	122.33	128.58
3	A	1335	NDP	C6A-C5A-N7A	-4.04	124.31	132.09
3	O	7335	NDP	C6A-C5A-N7A	-4.02	124.34	132.09
3	B	2335	NDP	C6A-C5A-N7A	-3.98	124.42	132.09
3	B	2335	NDP	O3X-P2B-O2X	3.77	121.93	107.80
3	A	1335	NDP	O3X-P2B-O2X	3.76	121.90	107.80
3	O	7335	NDP	O3X-P2B-O2X	3.72	121.76	107.80
3	O	7335	NDP	C5A-C4A-N9A	-3.69	101.79	105.81
3	B	2335	NDP	C5A-C4A-N9A	-3.65	101.84	105.81
3	A	1335	NDP	C5A-C4A-N9A	-3.61	101.88	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	7335	NDP	C2B-C1B-N9A	-3.37	108.21	113.75
3	B	2335	NDP	C2B-C1B-N9A	-3.36	108.23	113.75
3	A	1335	NDP	C2B-C1B-N9A	-3.34	108.26	113.75
3	A	1335	NDP	C6A-C5A-C4A	3.33	121.72	117.18
3	O	7335	NDP	C6A-C5A-C4A	3.29	121.67	117.18
3	B	2335	NDP	C6A-C5A-C4A	3.28	121.65	117.18
3	O	7335	NDP	C2A-N3A-C4A	3.27	119.82	111.83
3	A	1335	NDP	C2A-N3A-C4A	3.25	119.76	111.83
3	B	2335	NDP	C2A-N3A-C4A	3.21	119.68	111.83
3	B	2335	NDP	N9A-C8A-N7A	-3.03	109.63	113.94
3	O	7335	NDP	N9A-C8A-N7A	-3.03	109.64	113.94
3	A	1335	NDP	N9A-C8A-N7A	-2.98	109.71	113.94
3	O	7335	NDP	C4A-C5A-N7A	2.97	113.98	110.58
3	A	1335	NDP	C4A-C5A-N7A	2.97	113.97	110.58
3	B	2335	NDP	C4A-C5A-N7A	2.93	113.93	110.58
3	O	7335	NDP	O3D-C3D-C4D	-2.92	102.69	111.08
3	A	1335	NDP	O3D-C3D-C4D	-2.91	102.73	111.08
3	B	2335	NDP	O3D-C3D-C4D	-2.89	102.77	111.08
3	O	7335	NDP	C2D-C1D-N1N	2.85	120.31	113.31
3	A	1335	NDP	P2B-O2B-C2B	-2.57	116.57	123.43
3	B	2335	NDP	P2B-O2B-C2B	-2.52	116.69	123.43
3	O	7335	NDP	P2B-O2B-C2B	-2.51	116.73	123.43
3	O	7335	NDP	C1D-N1N-C6N	-2.36	115.79	120.77
3	A	1335	NDP	C1D-N1N-C6N	-2.32	115.87	120.77
3	B	2335	NDP	C1D-N1N-C6N	-2.29	115.93	120.77
3	O	7335	NDP	O5D-PN-O1N	-2.23	100.08	108.94
3	B	2335	NDP	O5D-PN-O1N	-2.23	100.10	108.94
3	A	1335	NDP	O2X-P2B-O1X	-2.23	102.17	110.83
3	A	1335	NDP	O5D-PN-O1N	-2.22	100.13	108.94
3	B	2335	NDP	O2X-P2B-O1X	-2.21	102.21	110.83
3	O	7335	NDP	O2X-P2B-O1X	-2.21	102.22	110.83
3	A	1335	NDP	N6A-C6A-N1A	2.19	123.25	118.38
3	O	7335	NDP	N6A-C6A-N1A	2.18	123.24	118.38
3	B	2335	NDP	N6A-C6A-N1A	2.17	123.20	118.38
3	B	2335	NDP	C3N-C2N-N1N	-2.13	120.07	123.20
3	O	7335	NDP	C3N-C2N-N1N	-2.11	120.10	123.20
3	B	2335	NDP	O4B-C1B-C2B	-2.07	103.03	106.59
3	A	1335	NDP	C3N-C2N-N1N	-2.06	120.19	123.20
3	O	7335	NDP	O4B-C1B-C2B	-2.04	103.07	106.59
3	A	1335	NDP	O4B-C1B-C2B	-2.03	103.09	106.59

There are no chirality outliers.

All (19) torsion outliers are listed below:

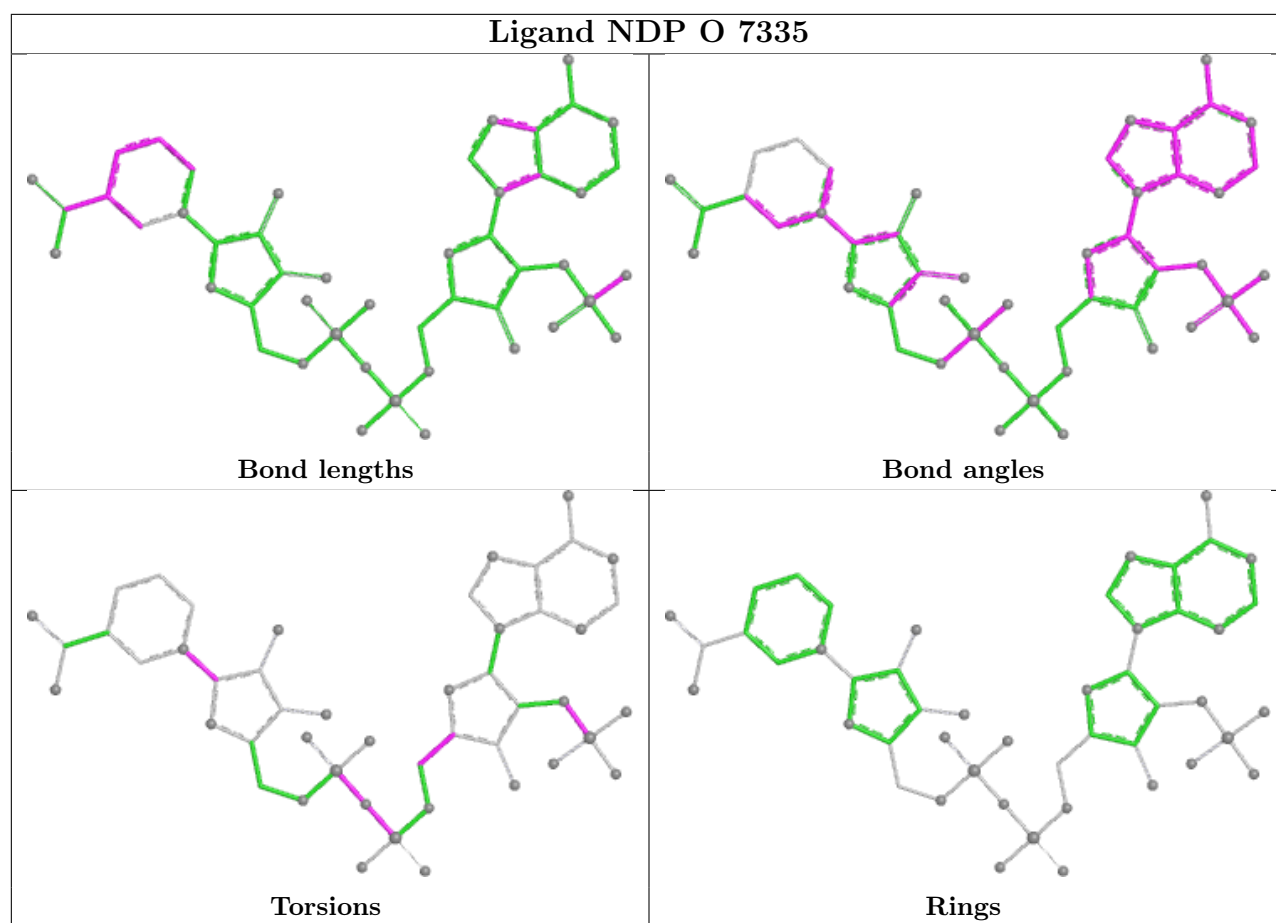
Mol	Chain	Res	Type	Atoms
3	A	1335	NDP	PN-O3-PA-O5B
3	O	7335	NDP	PN-O3-PA-O5B
3	A	1335	NDP	PA-O3-PN-O2N
3	O	7335	NDP	PA-O3-PN-O2N
3	O	7335	NDP	C2B-O2B-P2B-O2X
3	O	7335	NDP	O4D-C1D-N1N-C6N
3	A	1335	NDP	O4D-C1D-N1N-C6N
3	B	2335	NDP	O4D-C1D-N1N-C6N
3	O	7335	NDP	C2D-C1D-N1N-C6N
3	A	1335	NDP	C2D-C1D-N1N-C6N
3	B	2335	NDP	C2D-C1D-N1N-C6N
3	O	7335	NDP	PA-O3-PN-O1N
3	A	1335	NDP	PA-O3-PN-O1N
3	B	2335	NDP	PA-O3-PN-O2N
3	O	7335	NDP	O4B-C4B-C5B-O5B
3	A	1335	NDP	O4B-C4B-C5B-O5B
3	B	2335	NDP	O4B-C4B-C5B-O5B
3	B	2335	NDP	C2B-O2B-P2B-O2X
3	O	7335	NDP	O4D-C1D-N1N-C2N

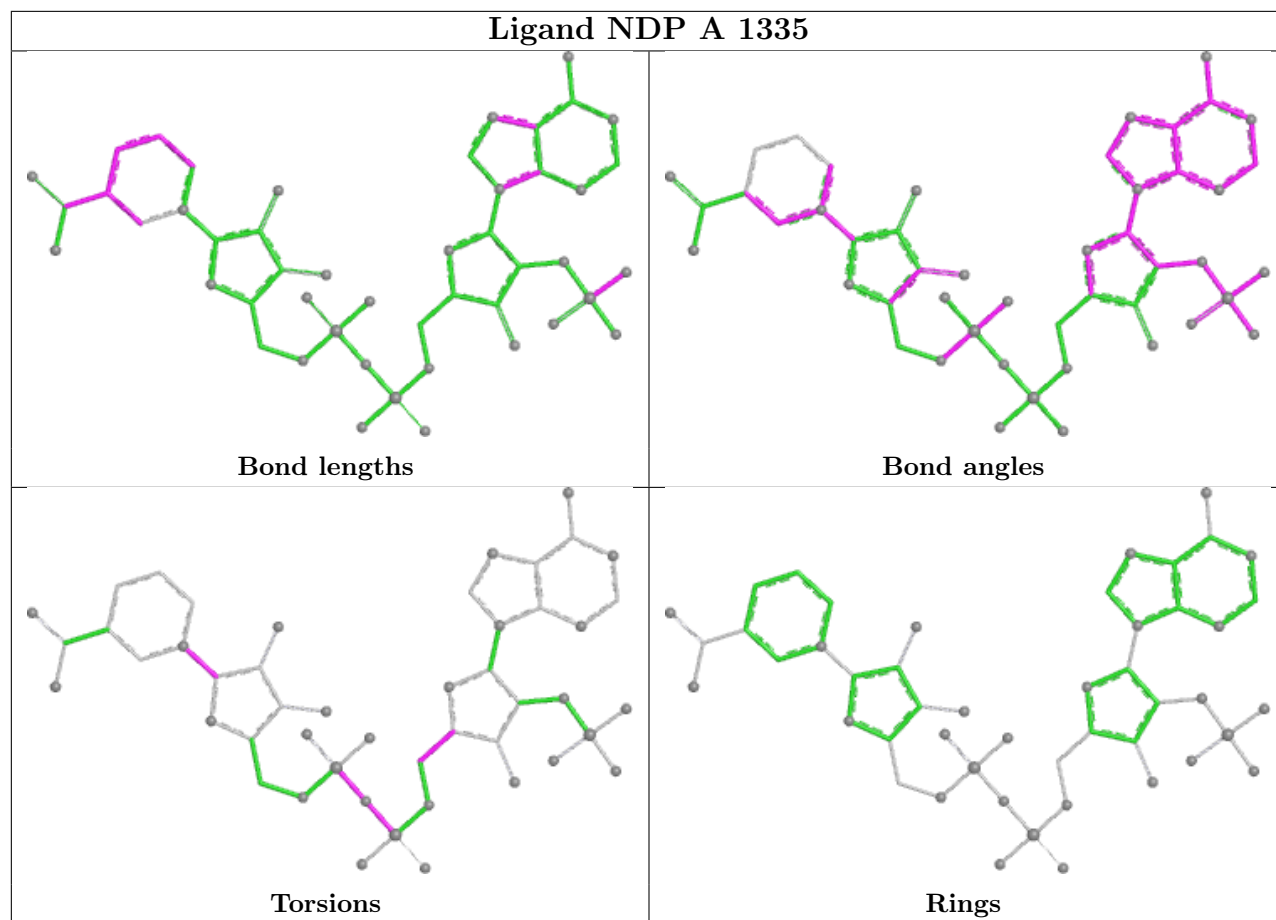
There are no ring outliers.

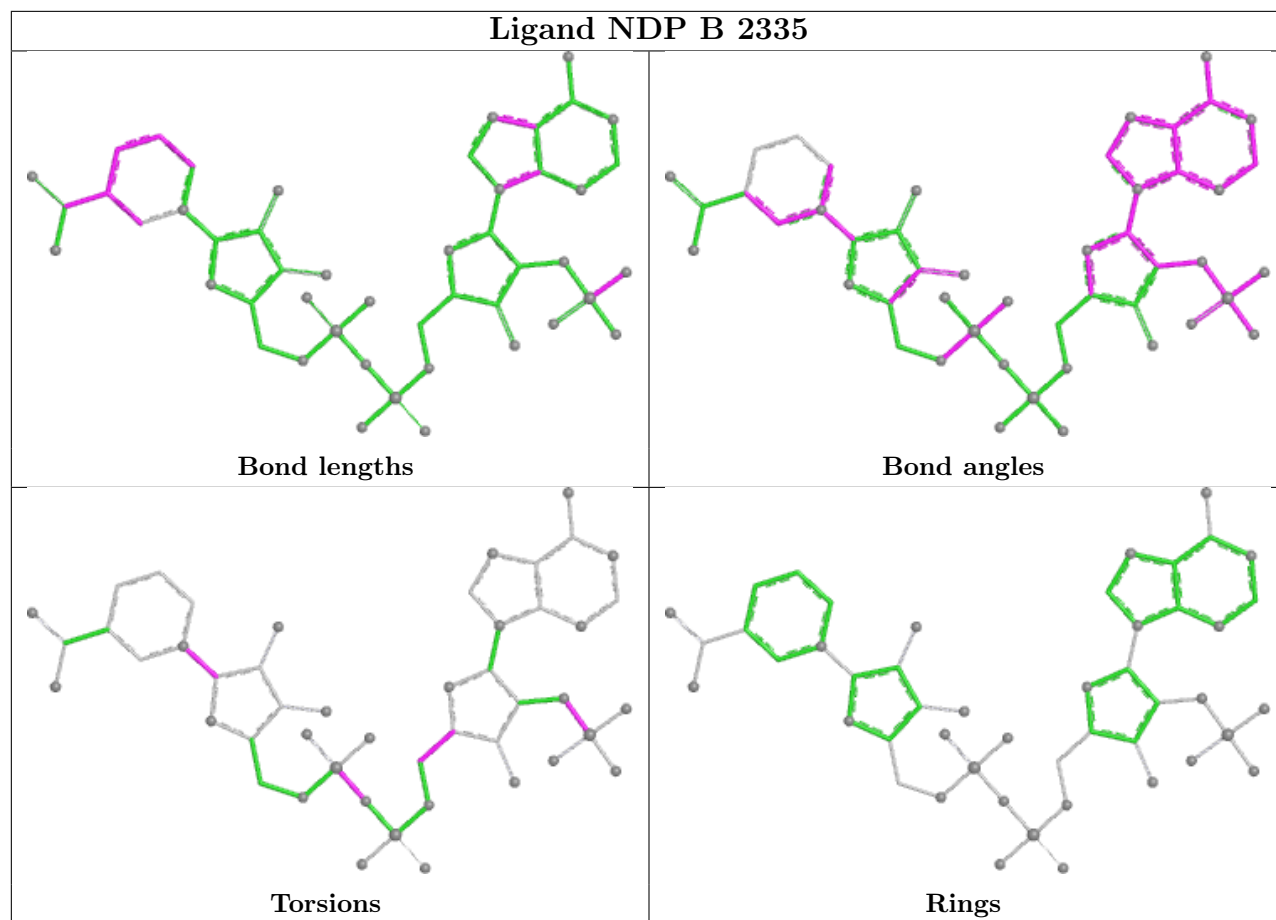
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2335	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	337/337 (100%)	1.07	54 (16%) 5 5	19, 32, 49, 58	4 (1%)
1	B	337/337 (100%)	1.31	96 (28%) 1 1	16, 35, 67, 87	4 (1%)
1	O	337/337 (100%)	0.13	8 (2%) 59 62	8, 20, 34, 55	10 (2%)
All	All	1011/1011 (100%)	0.84	158 (15%) 5 5	8, 28, 59, 87	18 (1%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	9.5
1	O	334	ALA	8.7
1	B	332	TRP	7.1
1	B	334	ALA	6.6
1	B	81	ASN	5.8
1	B	37	VAL	5.2
1	B	38	LYS	5.1
1	B	62	SER	5.0
1	B	61	ASP	4.6
1	B	80	VAL	4.6
1	A	252	ALA	4.4
1	B	82	LEU	4.4
1	B	113	ALA	4.3
1	A	253	GLU	4.3
1	B	77	ARG	4.2
1	B	333	GLN	4.2
1	B	64	ILE	4.1
1	B	71	ILE	4.1
1	A	22	ASP	4.0
1	A	163	GLN	4.0
1	A	226[A]	ASN	3.9
1	A	299	VAL	3.9
1	B	89	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	3.8
1	B	103	ASP	3.8
1	B	67	ASP	3.7
1	B	60	ALA	3.7
1	B	22	ASP	3.7
1	B	3	VAL	3.6
1	A	250	THR	3.6
1	B	83	PRO	3.6
1	A	211	ALA	3.5
1	B	66	VAL	3.5
1	B	111	ALA	3.5
1	B	65	SER	3.5
1	B	56[A]	ASP	3.5
1	A	258	ALA	3.4
1	B	76	ASP	3.4
1	O	135	GLU	3.4
1	B	114	LYS	3.4
1	B	0	LYS	3.3
1	B	75	SER	3.3
1	A	244	VAL	3.3
1	B	106	GLY	3.2
1	B	63	ALA	3.2
1	O	0	LYS	3.2
1	B	30	ILE	3.2
1	B	58	LYS	3.2
1	O	333	GLN	3.2
1	B	32	ASP	3.1
1	B	23	SER	3.1
1	O	124	ASP	3.1
1	A	255	VAL	3.1
1	B	70	VAL	3.1
1	B	72	LYS	3.1
1	B	85	GLY	3.0
1	B	191	ARG	3.0
1	B	26	ASP	3.0
1	B	102	ARG	3.0
1	A	191	ARG	3.0
1	B	69	LYS	3.0
1	B	78	ASN	2.9
1	A	225	LEU	2.9
1	A	124	ASP	2.9
1	B	73	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	122(A)	LYS	2.9
1	A	303	ASP	2.8
1	A	309	ALA	2.8
1	B	1	LEU	2.8
1	B	135	GLU	2.8
1	A	228	ILE	2.8
1	B	36	GLY	2.8
1	B	60(A)	GLY	2.8
1	B	79	PRO	2.8
1	B	74	VAL	2.8
1	B	123	GLY	2.7
1	B	109	LEU	2.7
1	B	330	ASN	2.7
1	B	100	VAL	2.7
1	A	301	GLY	2.7
1	B	55	ALA	2.6
1	B	59	THR	2.6
1	A	212	LYS	2.6
1	B	2	LYS	2.6
1	B	124	ASP	2.6
1	A	164	LYS	2.6
1	B	110	GLN	2.5
1	A	246	VAL	2.5
1	B	27	VAL	2.5
1	B	21	LYS	2.5
1	B	4	ALA	2.5
1	B	140	ALA	2.5
1	B	216	LEU	2.5
1	A	304	MET	2.5
1	A	158	VAL	2.5
1	B	98	VAL	2.5
1	B	187	ALA	2.5
1	B	7	GLY	2.5
1	B	122	GLY	2.5
1	B	20	ARG	2.4
1	B	34	GLY	2.4
1	O	61	ASP	2.4
1	A	295	SER	2.4
1	A	300[A]	MET	2.4
1	B	138	THR	2.4
1	B	331	LYS	2.4
1	B	121	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	108	HIS	2.4
1	A	257	ALA	2.4
1	B	101	ASP	2.4
1	A	172	MET	2.4
1	A	218	LEU	2.3
1	O	191	ARG	2.3
1	A	240	VAL	2.3
1	B	88	GLY	2.3
1	B	86	ASP	2.3
1	A	153	CYS	2.3
1	A	135	GLU	2.3
1	A	261	GLU	2.3
1	A	168	ILE	2.3
1	A	277	PRO	2.2
1	A	213	ALA	2.2
1	B	87	MET	2.2
1	A	251	PHE	2.2
1	A	21	LYS	2.2
1	A	122(A)	LYS	2.2
1	A	219	PRO	2.2
1	B	57	VAL	2.2
1	A	120	ALA	2.2
1	B	117	LEU	2.2
1	A	333	GLN	2.2
1	B	139	HIS	2.2
1	A	0	LYS	2.2
1	B	99	PHE	2.2
1	O	211	ALA	2.2
1	B	90	ASP	2.2
1	B	127	THR	2.2
1	A	132	VAL	2.1
1	A	245	GLN	2.1
1	A	216	LEU	2.1
1	A	221	LEU	2.1
1	A	302	ASP	2.1
1	B	125	ILE	2.1
1	B	107	LYS	2.1
1	B	115	LYS	2.1
1	B	46	TYR	2.1
1	B	5	ILE	2.1
1	A	165	PHE	2.1
1	B	105	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	39	GLN	2.1
1	A	223	GLY	2.1
1	A	169	LYS	2.1
1	B	328	VAL	2.1
1	A	266	GLU	2.0
1	B	212	LYS	2.0
1	A	307	VAL	2.0
1	A	222	LYS	2.0
1	B	126	PRO	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](#)

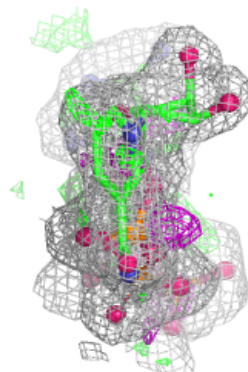
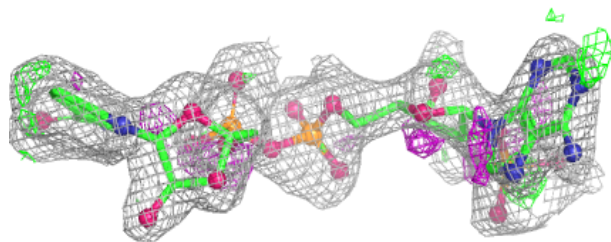
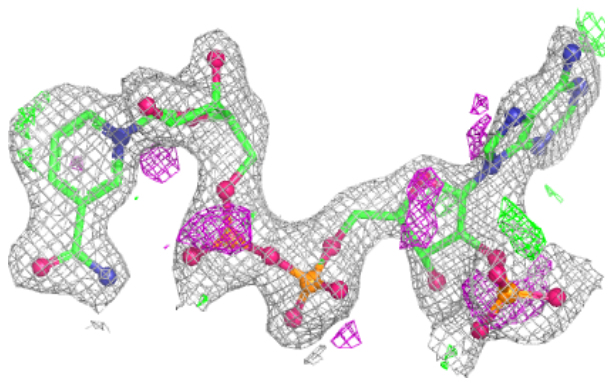
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	O	902	5/5	0.79	0.22	41,44,45,45	5
2	SO4	B	904	5/5	0.79	0.22	84,84,84,84	5
2	SO4	B	2339	5/5	0.80	0.20	62,63,63,63	0
2	SO4	A	1339	5/5	0.84	0.18	62,63,64,64	0
2	SO4	A	903	5/5	0.84	0.22	70,70,71,71	5
2	SO4	O	7339	5/5	0.85	0.17	59,59,59,60	0
3	NDP	B	2335	48/48	0.85	0.17	35,43,65,66	0
3	NDP	A	1335	48/48	0.86	0.16	23,33,47,50	0
2	SO4	A	1338	5/5	0.89	0.16	63,64,64,64	0
2	SO4	A	901	5/5	0.90	0.13	56,57,57,58	5
3	NDP	O	7335	48/48	0.90	0.13	15,24,44,49	0
2	SO4	B	2338	5/5	0.91	0.12	61,61,62,62	0
2	SO4	O	7338	5/5	0.97	0.10	34,35,37,37	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.

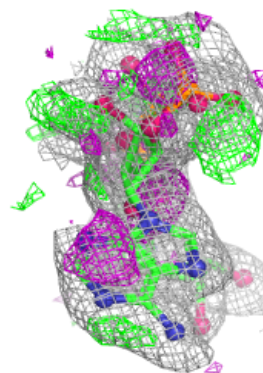
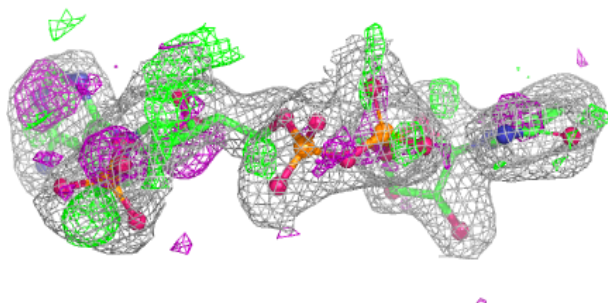
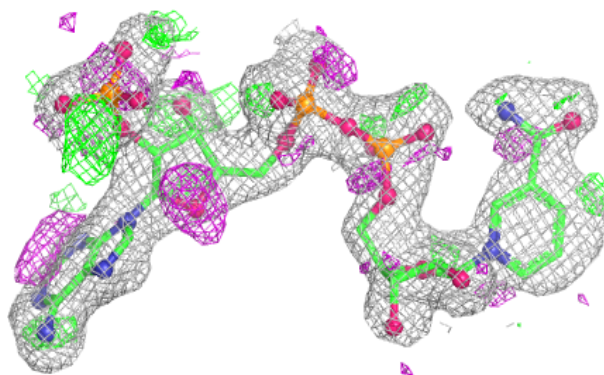
Electron density around NDP B 2335:

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

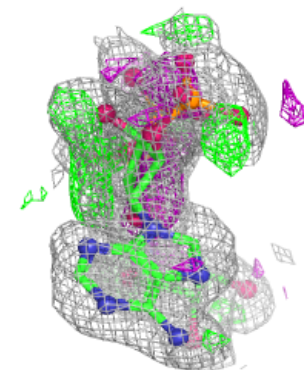
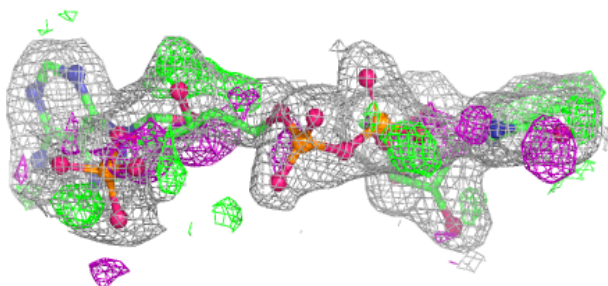
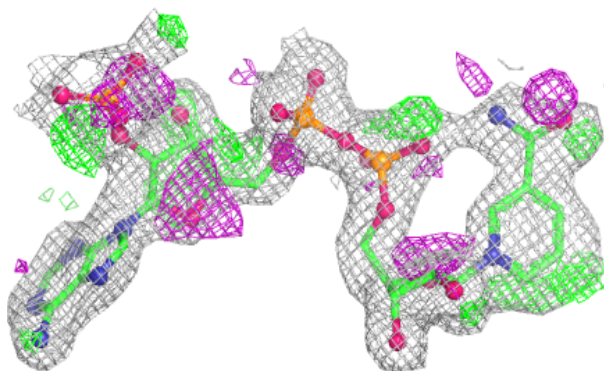


Electron density around NDP A 1335:

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

**Electron density around NDP O 7335:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.