



Full wwPDB X-ray Structure Validation Report

Mar 8, 2026 – 12:36 AM UTC

PDB ID : 2DBV / pdb_00002dbv
Title : GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE MUTANT WITH ASP 32 REPLACED BY GLY, LEU 187 REPLACED BY ALA, AND PRO 188 REPLACED BY SER COMPLEXED WITH NADP+
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Deposited on : 1996-12-19
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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

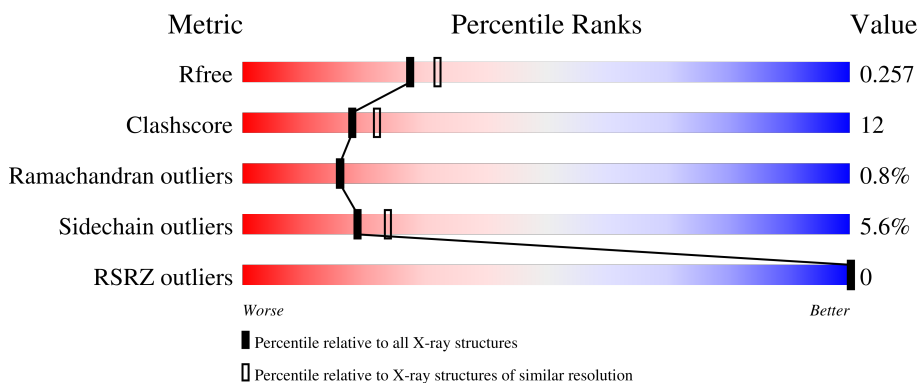
1 Overall quality at a glance i

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	O	334	 68% 29% .
1	P	334	 66% 29% 5% .
1	Q	334	 70% 28% .
1	R	334	 69% 29% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10693 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	334	2517	1575	445	488	9	0	0	0
1	P	334	2517	1575	445	488	9	0	0	0
1	Q	334	2517	1575	445	488	9	0	0	0
1	R	334	2517	1575	445	488	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	32	GLY	ASP	engineered mutation	UNP P00362
O	187	ALA	LEU	engineered mutation	UNP P00362
O	188	SER	PRO	engineered mutation	UNP P00362
P	32	GLY	ASP	engineered mutation	UNP P00362
P	187	ALA	LEU	engineered mutation	UNP P00362
P	188	SER	PRO	engineered mutation	UNP P00362
Q	32	GLY	ASP	engineered mutation	UNP P00362
Q	187	ALA	LEU	engineered mutation	UNP P00362
Q	188	SER	PRO	engineered mutation	UNP P00362
R	32	GLY	ASP	engineered mutation	UNP P00362
R	187	ALA	LEU	engineered mutation	UNP P00362
R	188	SER	PRO	engineered mutation	UNP P00362

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



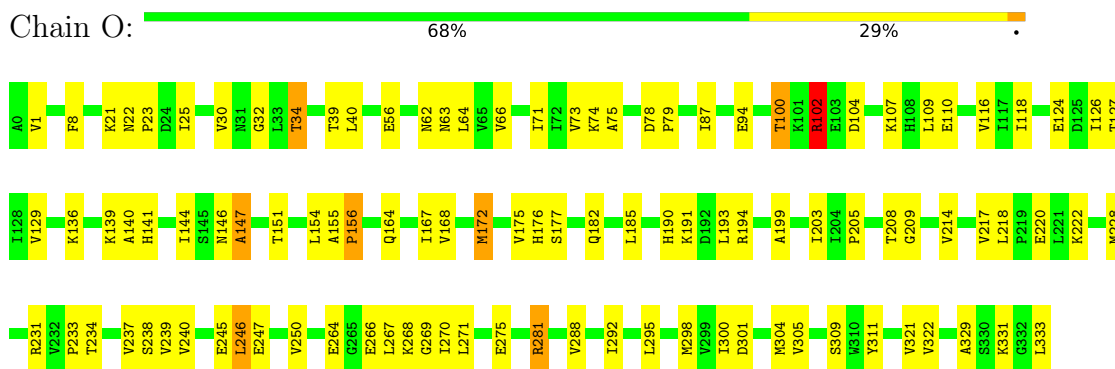
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

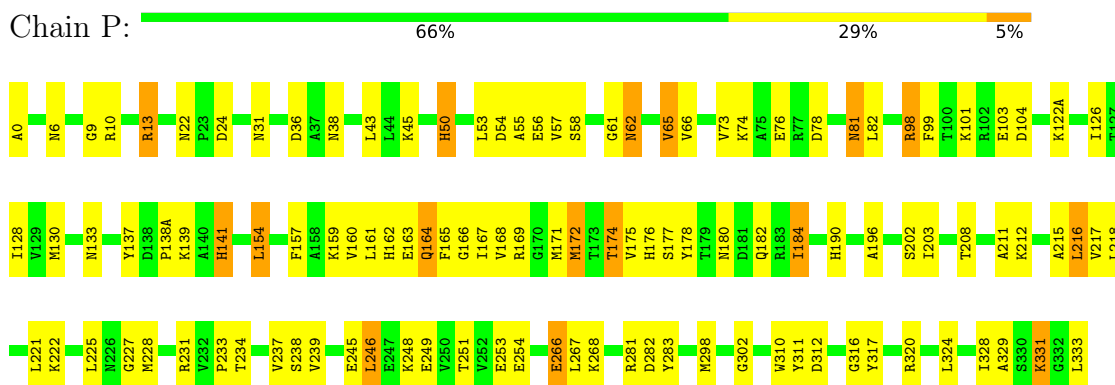
3 Residue-property plots [i](#)

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.

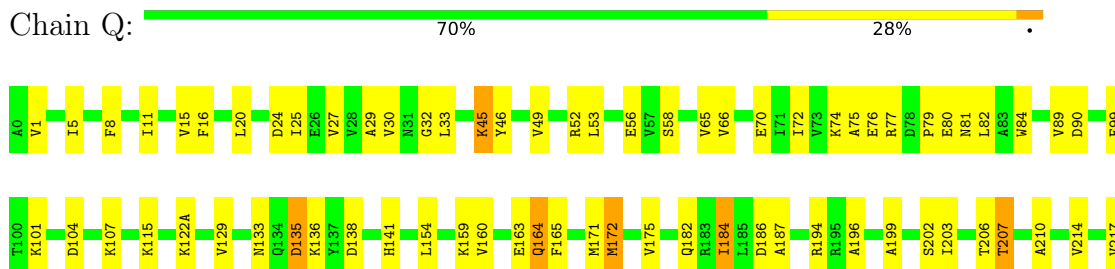
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



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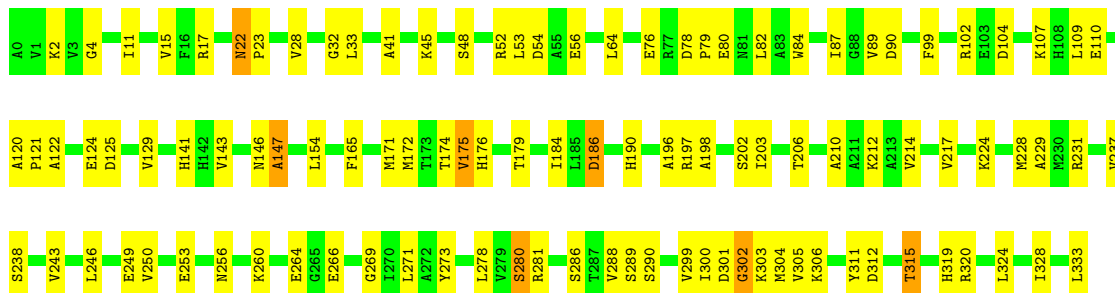
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





● Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain R: 69% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 124.27Å 82.45Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.8 (8.00-2.20) 83.9 (8.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.21Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.265 0.197 , 0.257	Depositor DCC
R_{free} test set	6666 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.440 for l,-k,h	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10693	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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 i

5.1 Standard geometry i

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	O	0.72	0/2552	1.13	16/3460 (0.5%)
1	P	0.74	0/2552	1.14	20/3460 (0.6%)
1	Q	0.74	1/2552 (0.0%)	1.13	10/3460 (0.3%)
1	R	0.75	1/2552 (0.0%)	1.14	15/3460 (0.4%)
All	All	0.73	2/10208 (0.0%)	1.14	61/13840 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	49	VAL	CA-CB	-5.46	1.49	1.55
1	R	84	TRP	NE1-CE2	-5.19	1.31	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	203	ILE	N-CA-C	-10.62	93.29	108.58
1	P	203	ILE	N-CA-C	-8.91	94.99	107.99
1	Q	175	VAL	N-CA-C	-8.31	94.77	107.73
1	O	203	ILE	N-CA-C	-7.87	96.18	108.23
1	O	164	GLN	N-CA-C	7.62	119.48	111.03
1	O	199	ALA	N-CA-C	7.58	119.18	111.07
1	O	175	VAL	N-CA-C	-7.31	95.96	107.15
1	R	22	ASN	CA-C-N	6.82	126.44	119.56
1	R	22	ASN	C-N-CA	6.82	126.44	119.56
1	Q	203	ILE	N-CA-C	-6.80	97.82	108.23
1	R	312	ASP	N-CA-C	-6.78	98.16	108.67
1	P	175	VAL	N-CA-C	-6.70	97.28	107.73
1	R	315	THR	N-CA-C	6.64	118.31	111.14
1	P	233	PRO	N-CA-C	6.55	125.96	112.47
1	R	175	VAL	N-CA-C	-6.46	98.22	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	87	ILE	N-CA-C	6.43	118.45	111.77
1	Q	280	SER	N-CA-C	6.41	118.80	111.11
1	R	154	LEU	N-CA-C	6.39	118.04	111.14
1	R	109	LEU	N-CA-C	-6.29	104.50	111.36
1	Q	154	LEU	N-CA-C	6.28	117.92	111.14
1	P	61	GLY	N-CA-C	-5.95	99.08	113.18
1	O	190	HIS	N-CA-C	-5.83	99.66	108.52
1	P	154	LEU	N-CA-C	5.78	117.67	111.36
1	O	78	ASP	CA-C-N	5.77	127.06	119.84
1	O	78	ASP	C-N-CA	5.77	127.06	119.84
1	Q	247	GLU	N-CA-C	-5.76	104.97	112.23
1	Q	199	ALA	N-CA-C	5.75	117.55	111.28
1	P	141	HIS	N-CA-C	5.73	117.86	108.52
1	O	209	GLY	N-CA-C	-5.67	105.93	115.80
1	O	102	ARG	N-CA-C	5.65	118.98	111.75
1	Q	45	LYS	N-CA-C	5.63	117.22	111.14
1	P	168	VAL	N-CA-C	-5.45	105.29	110.42
1	R	141	HIS	N-CA-C	5.44	117.39	108.52
1	P	22	ASN	CA-C-N	5.42	125.11	119.64
1	P	22	ASN	C-N-CA	5.42	125.11	119.64
1	R	4	GLY	N-CA-C	-5.41	101.99	111.46
1	O	233	PRO	N-CA-C	5.40	123.59	112.47
1	P	227	GLY	N-CA-C	5.39	119.01	111.19
1	O	154	LEU	N-CA-C	5.38	117.01	111.03
1	P	128	ILE	N-CA-C	5.36	116.20	108.48
1	P	234	THR	CA-C-N	5.36	124.87	119.19
1	P	234	THR	C-N-CA	5.36	124.87	119.19
1	P	65	VAL	N-CA-C	-5.35	99.85	107.77
1	O	140	ALA	N-CA-C	5.33	119.84	113.23
1	O	156	PRO	CA-C-N	-5.32	113.06	122.26
1	O	156	PRO	C-N-CA	-5.32	113.06	122.26
1	Q	233	PRO	N-CA-C	5.30	123.39	112.47
1	R	202	SER	N-CA-C	5.26	117.41	109.41
1	R	280	SER	N-CA-C	5.24	117.41	111.02
1	Q	227	GLY	N-CA-C	5.20	118.34	110.75
1	R	278	LEU	N-CA-C	5.14	118.05	110.59
1	Q	194	ARG	N-CA-C	-5.13	105.60	111.14
1	R	266	GLU	N-CA-C	5.12	118.31	111.75
1	P	50	HIS	CA-CB-CG	-5.10	108.70	113.80
1	R	210	ALA	N-CA-C	5.09	119.73	111.37
1	P	177	SER	N-CA-C	-5.08	103.83	110.53
1	P	316	GLY	N-CA-C	-5.06	106.63	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	312	ASP	N-CA-C	-5.05	99.55	108.23
1	P	331	LYS	N-CA-C	-5.04	107.10	113.20
1	O	321	VAL	N-CA-C	-5.03	105.64	110.72
1	P	202	SER	N-CA-C	5.02	116.62	109.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	O	2517	0	2563	60	0
1	P	2517	0	2563	75	0
1	Q	2517	0	2563	69	0
1	R	2517	0	2563	66	0
2	O	10	0	0	0	0
2	P	10	0	0	0	0
2	Q	10	0	0	1	0
2	R	10	0	0	0	0
3	O	48	0	26	2	0
3	P	48	0	26	3	0
3	Q	48	0	26	2	0
3	R	48	0	26	2	0
4	O	96	0	0	5	0
4	P	106	0	0	8	0
4	Q	87	0	0	1	0
4	R	104	0	0	2	0
All	All	10693	0	10356	252	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 12.

All (252) 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:300:ILE:HG22	1:O:304:MET:HB3	1.46	0.94
1:R:2:LYS:HE3	1:R:28:VAL:HG11	1.50	0.93
1:P:50:HIS:HD2	4:P:373:HOH:O	1.59	0.85
1:O:1:VAL:HG21	1:O:329:ALA:HB1	1.59	0.85
1:P:162:HIS:CD2	1:P:221:LEU:HD21	2.21	0.76
1:Q:76:GLU:HG2	1:Q:81:ASN:HB2	1.69	0.74
1:O:300:ILE:CG2	1:O:304:MET:HB3	2.18	0.74
1:Q:226:ASN:HB2	1:R:300:ILE:HD11	1.72	0.72
1:O:136:LYS:HE2	1:O:136:LYS:HA	1.70	0.72
1:R:17:ARG:HG2	1:R:53:LEU:HD13	1.72	0.71
1:O:8:PHE:HD2	1:O:40:LEU:HD22	1.55	0.71
1:O:298:MET:HB3	1:P:171:MET:HE1	1.71	0.71
1:Q:251:THR:OG1	1:Q:254:GLU:HG3	1.91	0.71
1:Q:25:ILE:HD13	1:Q:322:VAL:HG13	1.71	0.70
1:R:184:ILE:HD12	1:R:184:ILE:H	1.55	0.70
1:Q:165:PHE:HA	1:Q:248:LYS:HD3	1.73	0.69
1:Q:187:ALA:O	1:Q:196:ALA:HB1	1.92	0.69
1:P:98:ARG:HD3	4:P:409:HOH:O	1.92	0.68
1:P:176:HIS:HB3	1:P:231:ARG:HD3	1.75	0.68
1:P:184:ILE:HD11	1:Q:182:GLN:O	1.94	0.68
1:P:282:ASP:HB3	1:R:52:ARG:NH2	2.10	0.66
1:R:260:LYS:HE3	1:R:264:GLU:OE1	1.96	0.66
1:Q:136:LYS:HE2	1:Q:136:LYS:HA	1.77	0.65
1:O:1:VAL:HB	1:O:25:ILE:HG22	1.79	0.65
1:P:266:GLU:HG2	1:P:267:LEU:HG	1.78	0.64
1:R:32:GLY:O	1:R:33:LEU:HD23	1.98	0.64
1:O:56:GLU:O	1:O:66:VAL:HA	1.98	0.63
1:Q:80:GLU:HG2	1:Q:107:LYS:HD3	1.79	0.63
1:Q:298:MET:HB3	1:R:171:MET:HE1	1.79	0.63
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.34	0.62
1:P:218:LEU:HD13	1:P:221:LEU:HD12	1.80	0.62
1:Q:76:GLU:CG	1:Q:81:ASN:HB2	2.30	0.61
1:Q:160:VAL:O	1:Q:164:GLN:HB2	1.99	0.61
1:Q:226:ASN:CB	1:R:300:ILE:HD11	2.29	0.61
1:P:78:ASP:HB3	1:P:81:ASN:OD1	1.99	0.61
1:R:315:THR:O	1:R:319:HIS:HD2	1.83	0.61
1:Q:202:SER:OG	1:R:281:ARG:HG2	2.01	0.61
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.82	0.61
1:Q:129:VAL:HG23	1:Q:217:VAL:HG11	1.83	0.61
1:Q:76:GLU:HG2	1:Q:81:ASN:O	2.01	0.60
1:O:32:GLY:O	1:O:75:ALA:HA	2.03	0.59
1:P:9:GLY:HA3	3:P:336:NDP:O5B	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:101:LYS:HG2	1:Q:122(A):LYS:HD2	1.85	0.58
1:Q:136:LYS:HE2	1:Q:136:LYS:CA	2.34	0.58
1:P:320:ARG:NE	1:P:320:ARG:HA	2.17	0.58
1:Q:306:LYS:HE2	1:R:228:MET:HG2	1.87	0.57
1:Q:11:ILE:HD11	3:Q:336:NDP:H42N	1.87	0.57
1:R:249:GLU:HA	1:R:302:GLY:O	2.05	0.56
1:O:266:GLU:HG3	1:O:267:LEU:HG	1.86	0.56
1:P:163:GLU:HB2	1:P:164:GLN:NE2	2.20	0.56
1:R:79:PRO:HD2	1:R:107:LYS:NZ	2.21	0.56
1:Q:16:PHE:CE1	1:Q:20:LEU:HD21	2.41	0.56
1:R:176:HIS:O	1:R:231:ARG:HA	2.06	0.56
1:O:79:PRO:HG2	1:O:107:LYS:HD3	1.87	0.56
1:O:126:ILE:HD12	1:O:141:HIS:CE1	2.41	0.56
1:R:260:LYS:HD3	1:R:273:TYR:CD2	2.41	0.56
1:R:122:ALA:HB3	1:R:124:GLU:HB3	1.89	0.55
1:O:8:PHE:CD2	1:O:40:LEU:HD22	2.38	0.55
1:P:62:ASN:O	1:P:73:VAL:HB	2.07	0.55
1:P:180:ASN:HA	1:Q:184:ILE:HD12	1.89	0.55
1:Q:84:TRP:HB3	1:Q:89:VAL:HB	1.90	0.54
1:Q:300:ILE:HG22	1:Q:304:MET:HB3	1.88	0.54
1:R:165:PHE:CD1	1:R:250:VAL:HG11	2.43	0.54
1:R:76:GLU:HB2	1:R:82:LEU:CD2	2.38	0.54
1:P:10:ARG:NH1	1:Q:186:ASP:HB2	2.23	0.54
1:R:11:ILE:O	1:R:15:VAL:HG23	2.08	0.53
1:P:53:LEU:HD23	1:P:57:VAL:CG2	2.39	0.53
1:P:101:LYS:HB3	1:P:103:GLU:OE1	2.09	0.53
1:O:240:VAL:HG23	1:O:311:TYR:CE1	2.43	0.53
1:P:162:HIS:CD2	1:P:167:ILE:H	2.26	0.53
1:R:129:VAL:HG23	1:R:217:VAL:HG11	1.91	0.53
1:P:58:SER:OG	1:P:65:VAL:HB	2.09	0.53
1:P:101:LYS:HE3	4:P:345:HOH:O	2.08	0.53
1:Q:329:ALA:HA	1:Q:333:LEU:HD13	1.91	0.52
1:R:90:ASP:HB3	1:R:333:LEU:HD23	1.92	0.52
1:P:0:ALA:N	1:P:24:ASP:O	2.43	0.52
1:P:320:ARG:HA	1:P:320:ARG:HE	1.75	0.52
1:P:329:ALA:HA	1:P:333:LEU:HD22	1.90	0.52
1:P:103:GLU:H	1:P:103:GLU:CD	2.17	0.52
1:O:177:SER:HB3	1:O:234:THR:O	2.10	0.51
1:P:281:ARG:NH1	4:P:429:HOH:O	2.41	0.51
1:P:76:GLU:HB2	1:P:82:LEU:HD23	1.93	0.51
1:P:282:ASP:HB3	1:R:52:ARG:HH21	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:99:PHE:HD1	1:R:104:ASP:HB3	1.74	0.51
1:Q:305:VAL:HG22	1:Q:306:LYS:N	2.25	0.51
3:O:336:NDP:H1B	4:O:423:HOH:O	2.10	0.51
1:P:74:LYS:HE3	1:P:82:LEU:O	2.11	0.51
1:Q:5:ILE:HB	1:Q:30:VAL:HG12	1.91	0.50
1:Q:300:ILE:CG2	1:Q:304:MET:HB3	2.41	0.50
1:P:211:ALA:HB3	4:P:350:HOH:O	2.11	0.50
1:O:194:ARG:HD2	1:O:205:PRO:O	2.12	0.50
1:O:269:GLY:O	1:O:288:VAL:HG12	2.12	0.50
1:Q:115:LYS:NZ	1:Q:141:HIS:O	2.41	0.50
1:Q:206:THR:HG23	1:Q:229:ALA:HB3	1.92	0.50
1:R:146:ASN:O	1:R:147:ALA:HB3	2.12	0.50
1:R:315:THR:O	1:R:319:HIS:CD2	2.65	0.50
1:P:161:LEU:O	1:P:165:PHE:HB2	2.12	0.49
1:O:301:ASP:HB2	1:P:169:ARG:HD3	1.94	0.49
1:P:36:ASP:OD2	1:P:38:ASN:HB2	2.12	0.49
1:R:328:ILE:HG22	1:R:333:LEU:HD11	1.95	0.49
1:P:190:HIS:HB3	1:P:196:ALA:HB2	1.94	0.49
1:Q:207:THR:HG22	4:Q:381:HOH:O	2.11	0.49
1:Q:29:ALA:HB2	1:Q:72:ILE:HB	1.94	0.49
1:O:172:MET:HE2	1:O:208:THR:HG21	1.94	0.49
1:Q:99:PHE:HB3	1:Q:104:ASP:HB3	1.95	0.49
1:O:264:GLU:HA	1:O:268:LYS:HD3	1.95	0.49
1:R:212:LYS:HD3	4:R:355:HOH:O	2.12	0.49
1:P:6:ASN:OD1	1:P:31:ASN:HB3	2.12	0.49
1:P:138(A):PRO:HG2	1:P:139:LYS:HD2	1.95	0.49
1:Q:29:ALA:CB	1:Q:72:ILE:HB	2.42	0.49
1:Q:56:GLU:O	1:Q:66:VAL:HA	2.13	0.48
1:R:190:HIS:HB3	1:R:196:ALA:HB2	1.95	0.48
1:R:238:SER:HB2	1:R:311:TYR:CZ	2.48	0.48
1:P:238:SER:HB2	1:P:311:TYR:CZ	2.48	0.48
1:R:76:GLU:HB2	1:R:82:LEU:HD21	1.95	0.48
1:O:94:GLU:HG3	4:O:357:HOH:O	2.12	0.48
1:P:249:GLU:HA	1:P:302:GLY:O	2.14	0.48
1:R:41:ALA:HB2	1:R:64:LEU:HD22	1.96	0.48
1:Q:33:LEU:HD11	3:Q:336:NDP:C5A	2.43	0.48
1:O:222:LYS:HD3	1:O:222:LYS:C	2.39	0.47
1:P:56:GLU:O	1:P:66:VAL:HA	2.15	0.47
1:O:144:ILE:HD12	1:O:144:ILE:H	1.79	0.47
1:Q:79:PRO:HA	1:Q:82:LEU:HD12	1.95	0.47
1:O:100:THR:HG22	1:O:118:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:43:LEU:HA	4:P:344:HOH:O	2.15	0.47
1:P:76:GLU:HB2	1:P:82:LEU:CD2	2.44	0.47
1:Q:74:LYS:HE2	1:Q:82:LEU:O	2.15	0.47
1:O:167:ILE:HG12	1:O:246:LEU:CD1	2.45	0.47
1:Q:249:GLU:HA	1:Q:302:GLY:O	2.15	0.47
1:R:120:ALA:HB2	3:R:336:NDP:O3D	2.14	0.47
1:R:186:ASP:HA	1:R:196:ALA:O	2.15	0.47
1:O:62:ASN:O	1:O:73:VAL:HB	2.15	0.47
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.97	0.47
1:P:216:LEU:N	1:P:216:LEU:HD23	2.30	0.47
1:Q:202:SER:HB3	1:R:280:SER:OG	2.15	0.47
1:R:107:LYS:O	1:R:110:GLU:HB2	2.14	0.47
1:R:269:GLY:O	1:R:288:VAL:HG12	2.15	0.47
1:O:107:LYS:O	1:O:110:GLU:HB2	2.15	0.46
1:Q:45:LYS:O	1:Q:52:ARG:HA	2.16	0.46
1:O:151:THR:HG23	1:O:214:VAL:HG22	1.96	0.46
1:O:146:ASN:O	1:O:147:ALA:HB3	2.15	0.46
1:O:228:MET:HE3	1:O:228:MET:HB2	1.85	0.46
1:Q:82:LEU:HD13	1:Q:84:TRP:HZ2	1.77	0.46
1:R:299:VAL:HG13	1:R:304:MET:O	2.15	0.46
1:P:99:PHE:HB3	1:P:104:ASP:HB3	1.97	0.46
1:P:281:ARG:HG2	1:R:48:SER:O	2.16	0.46
1:Q:172:MET:HA	1:Q:241:ASP:O	2.16	0.46
1:O:104:ASP:O	1:O:107:LYS:HD2	2.15	0.46
1:Q:282:ASP:CG	1:R:197:ARG:HH22	2.23	0.46
1:O:168:VAL:HG22	1:O:247:GLU:HG3	1.98	0.46
1:O:271:LEU:HD11	1:O:292:ILE:HG12	1.97	0.46
1:O:176:HIS:HA	1:O:238:SER:HB3	1.98	0.45
1:O:182:GLN:HB3	4:O:360:HOH:O	2.16	0.45
1:R:271:LEU:HD12	1:R:290:SER:HB3	1.98	0.45
1:R:289:SER:OG	1:R:320:ARG:HD2	2.16	0.45
1:O:239:VAL:HG23	1:O:309:SER:O	2.14	0.45
1:P:283:TYR:CE2	1:P:310:TRP:CD1	3.05	0.45
1:R:253:GLU:CD	1:R:253:GLU:H	2.23	0.45
1:O:264:GLU:HA	1:O:268:LYS:CD	2.46	0.45
1:P:178:TYR:HA	1:P:182:GLN:OE1	2.17	0.45
1:R:243:VAL:HA	1:R:305:VAL:O	2.15	0.45
1:Q:210:ALA:HB2	2:Q:339:SO4:O1	2.17	0.45
1:Q:218:LEU:HB3	1:Q:221:LEU:HD12	1.98	0.45
1:R:249:GLU:HG2	1:R:303:LYS:HG3	1.98	0.45
1:P:159:LYS:O	1:P:163:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:270:ILE:O	1:O:288:VAL:HB	2.17	0.45
1:O:64:LEU:HB2	1:O:71:ILE:HB	1.99	0.45
1:O:245:GLU:HG3	1:P:245:GLU:OE2	2.17	0.45
1:P:166:GLY:O	1:P:246:LEU:HA	2.17	0.45
1:Q:226:ASN:HB2	1:R:300:ILE:CD1	2.44	0.45
1:O:22:ASN:HD22	1:O:322:VAL:HG12	1.82	0.44
1:R:87:ILE:HG13	1:R:89:VAL:HG23	1.99	0.44
1:R:125:ASP:HB2	1:R:143:VAL:O	2.17	0.44
1:P:101:LYS:HG3	1:P:122(A):LYS:HE2	1.99	0.44
1:P:228:MET:HE3	1:P:228:MET:HB2	1.87	0.44
1:P:253:GLU:CD	1:P:253:GLU:H	2.25	0.44
1:O:1:VAL:HG21	1:O:329:ALA:CB	2.38	0.44
1:O:144:ILE:HD12	1:O:144:ILE:N	2.32	0.44
1:O:331:LYS:HA	1:O:331:LYS:HD3	1.64	0.44
1:P:281:ARG:NH2	4:P:385:HOH:O	2.51	0.44
1:Q:52:ARG:HH11	1:Q:52:ARG:HG2	1.82	0.44
1:P:154:LEU:HA	1:P:157:PHE:CE2	2.52	0.43
1:P:174:THR:HA	1:P:239:VAL:O	2.18	0.43
1:Q:90:ASP:HB3	1:Q:333:LEU:HD23	1.99	0.43
1:R:305:VAL:HG22	1:R:306:LYS:N	2.33	0.43
1:P:246:LEU:HD13	1:P:246:LEU:N	2.33	0.43
1:Q:159:LYS:O	1:Q:163:GLU:HG3	2.19	0.43
1:O:109:LEU:HD21	1:O:116:VAL:HG23	2.01	0.43
1:Q:16:PHE:CE2	1:Q:27:VAL:HG11	2.53	0.43
1:Q:165:PHE:O	1:Q:247:GLU:HB2	2.18	0.43
1:R:120:ALA:HB1	1:R:121:PRO:HD2	2.00	0.43
1:O:176:HIS:HB3	1:O:231:ARG:HD3	2.00	0.43
1:R:129:VAL:CG2	1:R:217:VAL:HG11	2.48	0.43
1:O:238:SER:HB2	1:O:311:TYR:CZ	2.53	0.43
1:P:137:TYR:HB3	4:P:393:HOH:O	2.19	0.43
1:O:34:THR:CG2	1:O:39:THR:HB	2.49	0.43
1:Q:45:LYS:HD2	1:Q:46:TYR:CZ	2.53	0.43
1:O:295:LEU:HG	4:O:350:HOH:O	2.18	0.42
1:P:215:ALA:HB2	1:P:222:LYS:HA	2.00	0.42
1:Q:133:ASN:C	1:Q:135:ASP:N	2.75	0.42
1:Q:230:MET:CE	1:R:175:VAL:HG21	2.48	0.42
1:R:41:ALA:O	1:R:45:LYS:HB2	2.19	0.42
1:Q:1:VAL:HG12	1:Q:24:ASP:O	2.18	0.42
1:Q:32:GLY:O	1:Q:75:ALA:HA	2.19	0.42
1:P:54:ASP:O	1:P:55:ALA:HB2	2.20	0.42
1:R:206:THR:HG23	1:R:229:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:LEU:HD23	1:O:193:LEU:HA	1.87	0.42
1:P:10:ARG:HG2	3:P:336:NDP:O2A	2.19	0.42
1:R:146:ASN:HD22	1:R:324:LEU:HD22	1.85	0.42
1:R:228:MET:HE3	1:R:228:MET:HB2	1.95	0.42
1:O:32:GLY:HA2	3:O:336:NDP:N3A	2.34	0.42
1:O:167:ILE:HG12	1:O:246:LEU:HD12	2.02	0.41
1:P:160:VAL:O	1:P:164:GLN:NE2	2.53	0.41
1:P:298:MET:HE3	1:P:298:MET:HB2	1.94	0.41
1:Q:20:LEU:HD12	1:Q:53:LEU:HD11	2.02	0.41
1:Q:25:ILE:CD1	1:Q:322:VAL:HG13	2.45	0.41
1:Q:138:ASP:H	1:Q:141:HIS:CE1	2.36	0.41
1:P:251:THR:H	1:P:254:GLU:HB2	1.85	0.41
1:P:133:ASN:ND2	1:P:217:VAL:HA	2.35	0.41
1:R:79:PRO:HD2	1:R:107:LYS:HZ3	1.84	0.41
1:R:107:LYS:HA	1:R:110:GLU:CD	2.45	0.41
1:R:179:THR:OG1	1:R:231:ARG:NH2	2.53	0.41
1:Q:33:LEU:CD2	1:Q:77:ARG:HB3	2.49	0.41
1:P:126:ILE:HD12	1:P:141:HIS:CE1	2.55	0.41
1:Q:52:ARG:HG2	1:Q:52:ARG:NH1	2.35	0.41
1:Q:260:LYS:O	1:Q:264:GLU:HG3	2.20	0.41
1:R:22:ASN:HA	1:R:23:PRO:HD2	1.92	0.41
1:R:174:THR:HG23	1:R:174:THR:O	2.20	0.41
1:P:162:HIS:HD2	1:P:167:ILE:H	1.66	0.41
1:O:185:LEU:HD23	1:O:185:LEU:HA	1.93	0.41
1:O:281:ARG:HD3	1:O:281:ARG:HA	1.90	0.41
4:O:427:HOH:O	1:Q:52:ARG:HD2	2.20	0.41
1:P:130:MET:HE2	1:P:324:LEU:HA	2.02	0.41
1:Q:138:ASP:HB3	1:Q:141:HIS:CE1	2.56	0.41
1:O:102:ARG:HG3	1:O:124:GLU:HA	2.01	0.41
1:Q:16:PHE:CD2	1:Q:27:VAL:HG11	2.55	0.41
1:O:71:ILE:HD12	1:O:71:ILE:N	2.36	0.41
1:O:270:ILE:HG22	1:O:271:LEU:N	2.35	0.41
1:P:9:GLY:O	1:P:13:ARG:HB2	2.20	0.41
1:P:137:TYR:OH	1:P:328:ILE:HG23	2.21	0.41
1:R:11:ILE:HD11	3:R:336:NDP:H42N	2.03	0.41
1:P:45:LYS:HE2	1:P:45:LYS:HB2	1.90	0.41
1:P:10:ARG:HH11	1:Q:186:ASP:HB2	1.86	0.40
1:P:208:THR:HG22	1:P:228:MET:HA	2.03	0.40
1:R:56:GLU:HA	4:R:419:HOH:O	2.20	0.40
1:P:317:TYR:O	1:P:320:ARG:HB2	2.22	0.40
1:O:139:LYS:HD3	1:O:139:LYS:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:31:ASN:ND2	3:P:336:NDP:H2A	2.36	0.40
1:R:99:PHE:CD1	1:R:104:ASP:HB3	2.55	0.40
1:P:154:LEU:HD22	1:P:172:MET:SD	2.62	0.40
1:R:90:ASP:CB	1:R:333:LEU:HD23	2.51	0.40
1:R:197:ARG:O	1:R:198:ALA:C	2.63	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	O	332/334 (99%)	311 (94%)	18 (5%)	3 (1%)	14 14
1	P	332/334 (99%)	310 (93%)	20 (6%)	2 (1%)	21 23
1	Q	332/334 (99%)	306 (92%)	25 (8%)	1 (0%)	36 42
1	R	332/334 (99%)	314 (95%)	14 (4%)	4 (1%)	10 8
All	All	1328/1336 (99%)	1241 (93%)	77 (6%)	10 (1%)	16 16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	147	ALA
1	O	237	VAL
1	P	237	VAL
1	Q	237	VAL
1	R	147	ALA
1	R	237	VAL
1	R	186	ASP
1	P	266	GLU
1	R	302	GLY
1	O	23	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	270/270 (100%)	252 (93%)	18 (7%)	15	17
1	P	270/270 (100%)	255 (94%)	15 (6%)	19	24
1	Q	270/270 (100%)	253 (94%)	17 (6%)	16	19
1	R	270/270 (100%)	259 (96%)	11 (4%)	27	37
All	All	1080/1080 (100%)	1019 (94%)	61 (6%)	19	24

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	21	LYS
1	O	30	VAL
1	O	34	THR
1	O	63	ASN
1	O	74	LYS
1	O	100	THR
1	O	102	ARG
1	O	127	THR
1	O	172	MET
1	O	191	LYS
1	O	218	LEU
1	O	220	GLU
1	O	246	LEU
1	O	250	VAL
1	O	275	GLU
1	O	281	ARG
1	O	305	VAL
1	O	333	LEU
1	P	13	ARG
1	P	62	ASN
1	P	81	ASN
1	P	98	ARG
1	P	164	GLN
1	P	172	MET

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Mol	Chain	Res	Type
1	P	174	THR
1	P	184	ILE
1	P	212	LYS
1	P	216	LEU
1	P	225	LEU
1	P	246	LEU
1	P	248	LYS
1	P	268	LYS
1	P	331	LYS
1	Q	8	PHE
1	Q	15	VAL
1	Q	58	SER
1	Q	65	VAL
1	Q	70	GLU
1	Q	135	ASP
1	Q	164	GLN
1	Q	171	MET
1	Q	172	MET
1	Q	184	ILE
1	Q	207	THR
1	Q	214	VAL
1	Q	220	GLU
1	Q	230	MET
1	Q	246	LEU
1	Q	299	VAL
1	Q	333	LEU
1	R	54	ASP
1	R	78	ASP
1	R	80	GLU
1	R	102	ARG
1	R	172	MET
1	R	214	VAL
1	R	224	LYS
1	R	246	LEU
1	R	256	ASN
1	R	286	SER
1	R	301	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	146	ASN

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Mol	Chain	Res	Type
1	O	152	ASN
1	O	256	ASN
1	P	38	ASN
1	P	50	HIS
1	P	63	ASN
1	P	146	ASN
1	P	162	HIS
1	P	164	GLN
1	P	256	ASN
1	Q	81	ASN
1	Q	152	ASN
1	Q	256	ASN
1	R	63	ASN
1	R	81	ASN
1	R	123	ASN
1	R	146	ASN
1	R	152	ASN
1	R	256	ASN
1	R	319	HIS

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](#)

12 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	SO4	R	339	-	4,4,4	0.54	0	6,6,6	0.54	0
2	SO4	O	338	-	4,4,4	0.57	0	6,6,6	0.52	0
3	NDP	R	336	-	51,52,52	1.69	9 (17%)	71,80,80	1.80	15 (21%)
3	NDP	P	336	-	51,52,52	1.54	10 (19%)	71,80,80	1.97	15 (21%)
3	NDP	Q	336	-	51,52,52	1.61	7 (13%)	71,80,80	2.19	24 (33%)
2	SO4	P	338	-	4,4,4	0.84	0	6,6,6	0.63	0
2	SO4	R	338	-	4,4,4	0.82	0	6,6,6	0.21	0
2	SO4	O	339	-	4,4,4	0.50	0	6,6,6	0.34	0
2	SO4	Q	338	-	4,4,4	0.88	0	6,6,6	0.45	0
2	SO4	Q	339	-	4,4,4	0.54	0	6,6,6	0.34	0
2	SO4	P	339	-	4,4,4	0.46	0	6,6,6	0.99	0
3	NDP	O	336	-	51,52,52	1.56	8 (15%)	71,80,80	2.18	21 (29%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	R	336	-	-	8/34/77/77	0/5/5/5
3	NDP	P	336	-	-	6/34/77/77	0/5/5/5
3	NDP	Q	336	-	-	5/34/77/77	0/5/5/5
3	NDP	O	336	-	-	8/34/77/77	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	336	NDP	C4N-C3N	-5.70	1.39	1.50
3	Q	336	NDP	C4N-C3N	-5.51	1.39	1.50
3	R	336	NDP	C4N-C3N	-5.08	1.40	1.50
3	P	336	NDP	C4N-C3N	-4.39	1.41	1.50
3	R	336	NDP	PN-O3	4.19	1.64	1.59
3	O	336	NDP	P2B-O1X	4.12	1.63	1.50
3	R	336	NDP	P2B-O1X	4.11	1.63	1.50
3	Q	336	NDP	PN-O3	3.89	1.63	1.59
3	R	336	NDP	C4N-C5N	-3.84	1.39	1.49
3	P	336	NDP	P2B-O1X	3.76	1.62	1.50
3	O	336	NDP	C4N-C5N	-3.61	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	336	NDP	C7N-C3N	3.60	1.56	1.48
3	Q	336	NDP	C4N-C5N	-3.44	1.40	1.49
3	P	336	NDP	C5A-N7A	-3.18	1.33	1.39
3	Q	336	NDP	C5A-N7A	-3.13	1.33	1.39
3	O	336	NDP	C5A-N7A	-3.06	1.33	1.39
3	P	336	NDP	C7N-C3N	3.06	1.55	1.48
3	Q	336	NDP	P2B-O1X	3.02	1.59	1.50
3	O	336	NDP	C7N-C3N	2.98	1.55	1.48
3	R	336	NDP	C5A-N7A	-2.84	1.33	1.39
3	R	336	NDP	PA-O3	2.68	1.62	1.59
3	P	336	NDP	C2N-C3N	2.67	1.42	1.35
3	Q	336	NDP	C7N-C3N	2.67	1.54	1.48
3	P	336	NDP	C6N-C5N	2.55	1.40	1.33
3	Q	336	NDP	C4A-N9A	-2.55	1.32	1.37
3	R	336	NDP	C4A-N9A	-2.51	1.32	1.37
3	O	336	NDP	C4A-N9A	-2.40	1.32	1.37
3	P	336	NDP	C4N-C5N	-2.39	1.42	1.49
3	O	336	NDP	C6N-C5N	2.31	1.40	1.33
3	O	336	NDP	C2N-C3N	2.25	1.41	1.35
3	P	336	NDP	P2B-O3X	2.21	1.63	1.54
3	P	336	NDP	C4A-N9A	-2.17	1.33	1.37
3	P	336	NDP	PA-O3	-2.12	1.57	1.59
3	R	336	NDP	P2B-O2X	2.10	1.62	1.54

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	336	NDP	N3A-C4A-N9A	7.34	139.65	127.17
3	O	336	NDP	C5A-C4A-N3A	-5.98	118.48	126.72
3	R	336	NDP	C5A-C4A-N3A	-5.89	118.60	126.72
3	Q	336	NDP	N3A-C4A-N9A	5.81	137.06	127.17
3	Q	336	NDP	C5A-C4A-N3A	-5.56	119.06	126.72
3	P	336	NDP	N3A-C4A-N9A	5.55	136.61	127.17
3	P	336	NDP	O3-PA-O1A	-5.25	94.91	110.70
3	R	336	NDP	N3A-C4A-N9A	5.20	136.01	127.17
3	Q	336	NDP	O4B-C4B-C5B	-5.18	92.73	109.33
3	O	336	NDP	C4A-N9A-C8A	5.01	111.00	105.74
3	Q	336	NDP	N3A-C2A-N1A	-4.62	121.59	128.58
3	Q	336	NDP	C6A-C5A-C4A	4.61	123.48	117.18
3	P	336	NDP	C5A-C4A-N3A	-4.60	120.38	126.72
3	Q	336	NDP	C6A-C5A-N7A	-4.42	123.57	132.09
3	Q	336	NDP	O4B-C1B-C2B	-4.33	99.13	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	336	NDP	N3A-C2A-N1A	-4.28	122.10	128.58
3	O	336	NDP	N3A-C2A-N1A	-4.24	122.17	128.58
3	R	336	NDP	C6A-C5A-C4A	4.23	122.95	117.18
3	O	336	NDP	C4B-O4B-C1B	-4.17	100.25	109.47
3	P	336	NDP	C6A-C5A-N7A	-4.04	124.30	132.09
3	O	336	NDP	C6A-C5A-N7A	-3.98	124.42	132.09
3	R	336	NDP	N3A-C2A-N1A	-3.76	122.89	128.58
3	O	336	NDP	O3X-P2B-O2X	3.75	121.84	107.80
3	O	336	NDP	C5A-C4A-N9A	-3.62	101.86	105.81
3	Q	336	NDP	C2B-C1B-N9A	3.46	119.45	113.75
3	R	336	NDP	C6A-C5A-N7A	-3.43	125.47	132.09
3	P	336	NDP	C4A-C5A-N7A	3.42	114.49	110.58
3	P	336	NDP	O2A-PA-O3	3.37	116.38	107.27
3	R	336	NDP	C2B-C1B-N9A	3.33	119.23	113.75
3	O	336	NDP	C2B-C1B-N9A	-3.31	108.31	113.75
3	Q	336	NDP	C2A-N1A-C6A	3.28	124.12	118.73
3	O	336	NDP	C6A-C5A-C4A	3.27	121.65	117.18
3	O	336	NDP	C2A-N3A-C4A	3.24	119.75	111.83
3	Q	336	NDP	O3X-P2B-O2B	3.09	117.88	105.85
3	P	336	NDP	C4A-N9A-C8A	3.06	108.95	105.74
3	O	336	NDP	N9A-C8A-N7A	-3.00	109.67	113.94
3	Q	336	NDP	C4A-N9A-C8A	2.97	108.85	105.74
3	O	336	NDP	C4A-C5A-N7A	2.93	113.94	110.58
3	P	336	NDP	C6A-C5A-C4A	2.92	121.16	117.18
3	Q	336	NDP	C3N-C2N-N1N	-2.90	118.94	123.20
3	O	336	NDP	O3D-C3D-C4D	-2.90	102.76	111.08
3	R	336	NDP	C2A-N3A-C4A	2.88	118.87	111.83
3	Q	336	NDP	C4B-O4B-C1B	-2.86	103.14	109.47
3	P	336	NDP	P2B-O2B-C2B	-2.81	115.93	123.43
3	R	336	NDP	O4B-C1B-C2B	-2.78	101.81	106.59
3	Q	336	NDP	C2D-C3D-C4D	2.76	107.94	102.61
3	Q	336	NDP	C2A-N3A-C4A	2.73	118.50	111.83
3	Q	336	NDP	O2A-PA-O3	2.72	114.62	107.27
3	P	336	NDP	C4B-O4B-C1B	-2.67	103.58	109.47
3	R	336	NDP	O2X-P2B-O1X	-2.65	100.50	110.83
3	P	336	NDP	C2A-N3A-C4A	2.57	118.11	111.83
3	P	336	NDP	C5A-C4A-N9A	-2.56	103.02	105.81
3	O	336	NDP	P2B-O2B-C2B	-2.55	116.63	123.43
3	Q	336	NDP	O2N-PN-O3	2.54	114.15	107.27
3	P	336	NDP	C2A-N1A-C6A	2.48	122.81	118.73
3	R	336	NDP	C3D-C2D-C1D	-2.47	96.79	101.46
3	R	336	NDP	O4D-C1D-N1N	2.46	112.78	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	336	NDP	C3B-C2B-C1B	-2.36	98.28	102.81
3	R	336	NDP	C3N-C2N-N1N	-2.35	119.75	123.20
3	O	336	NDP	C1D-N1N-C6N	-2.32	115.86	120.77
3	Q	336	NDP	O3B-C3B-C4B	2.32	117.75	111.08
3	P	336	NDP	O7N-C7N-N7N	-2.25	117.85	122.89
3	O	336	NDP	O5D-PN-O1N	-2.24	100.07	108.94
3	O	336	NDP	O2X-P2B-O1X	-2.22	102.20	110.83
3	O	336	NDP	N6A-C6A-N1A	2.21	123.31	118.38
3	Q	336	NDP	O5B-C5B-C4B	-2.20	101.49	108.99
3	Q	336	NDP	C3D-C2D-C1D	-2.20	97.30	101.46
3	R	336	NDP	O5B-C5B-C4B	-2.16	101.65	108.99
3	O	336	NDP	C3N-C2N-N1N	-2.11	120.11	123.20
3	Q	336	NDP	C1D-N1N-C6N	-2.10	116.34	120.77
3	R	336	NDP	C2A-N1A-C6A	2.08	122.15	118.73
3	O	336	NDP	O4B-C1B-C2B	-2.08	103.01	106.59
3	Q	336	NDP	C4A-C5A-N7A	2.07	112.95	110.58
3	Q	336	NDP	O4B-C1B-N9A	2.06	112.04	108.09
3	R	336	NDP	O5D-PN-O1N	-2.05	100.79	108.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	336	NDP	C5B-O5B-PA-O1A
3	O	336	NDP	PN-O3-PA-O5B
3	R	336	NDP	C5B-O5B-PA-O1A
3	P	336	NDP	C3B-C2B-O2B-P2B
3	R	336	NDP	O4D-C4D-C5D-O5D
3	R	336	NDP	O4B-C4B-C5B-O5B
3	R	336	NDP	C3B-C4B-C5B-O5B
3	O	336	NDP	PA-O3-PN-O2N
3	Q	336	NDP	C2D-C1D-N1N-C6N
3	O	336	NDP	C5B-O5B-PA-O3
3	R	336	NDP	C5B-O5B-PA-O3
3	Q	336	NDP	O4D-C1D-N1N-C6N
3	Q	336	NDP	PA-O3-PN-O2N
3	O	336	NDP	O4D-C1D-N1N-C6N
3	R	336	NDP	O4D-C1D-N1N-C6N
3	P	336	NDP	O4B-C4B-C5B-O5B
3	P	336	NDP	O4D-C1D-N1N-C6N
3	R	336	NDP	C2D-C1D-N1N-C6N
3	P	336	NDP	C1B-C2B-O2B-P2B

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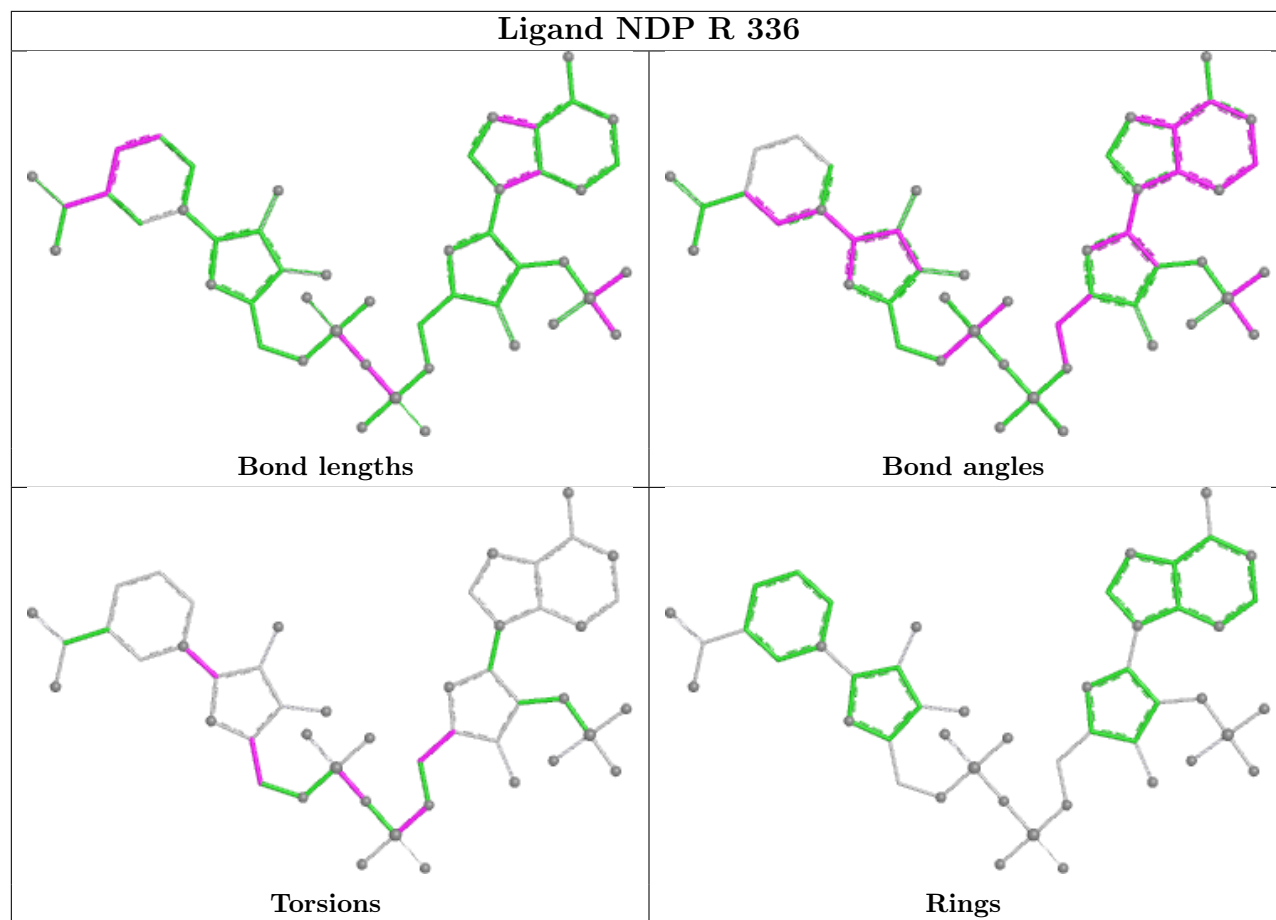
Mol	Chain	Res	Type	Atoms
3	O	336	NDP	C2D-C1D-N1N-C6N
3	P	336	NDP	C2D-C1D-N1N-C6N
3	O	336	NDP	O4B-C4B-C5B-O5B
3	O	336	NDP	PA-O3-PN-O1N
3	R	336	NDP	PA-O3-PN-O2N
3	P	336	NDP	C2N-C3N-C7N-O7N
3	Q	336	NDP	O4D-C1D-N1N-C2N
3	Q	336	NDP	PA-O3-PN-O1N

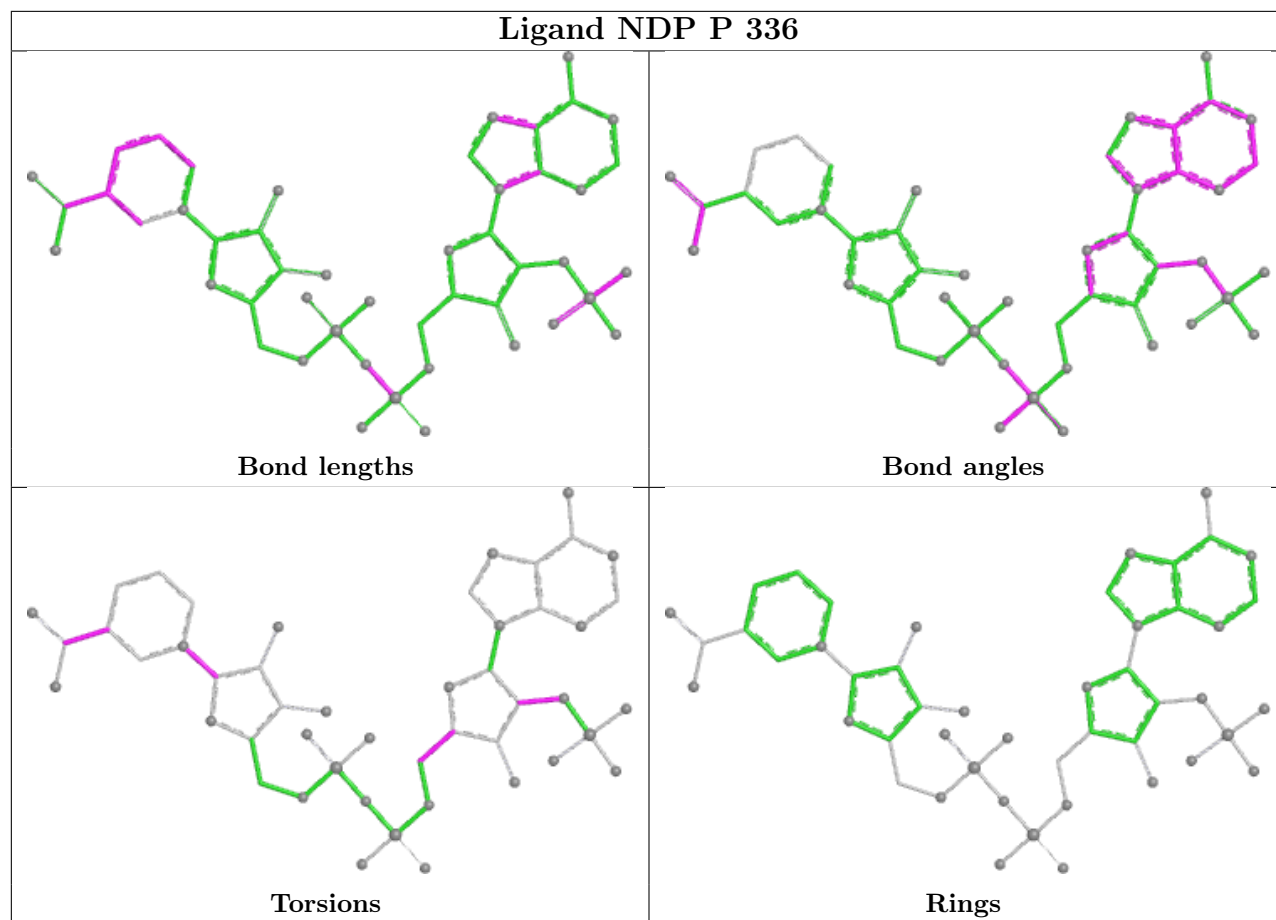
There are no ring outliers.

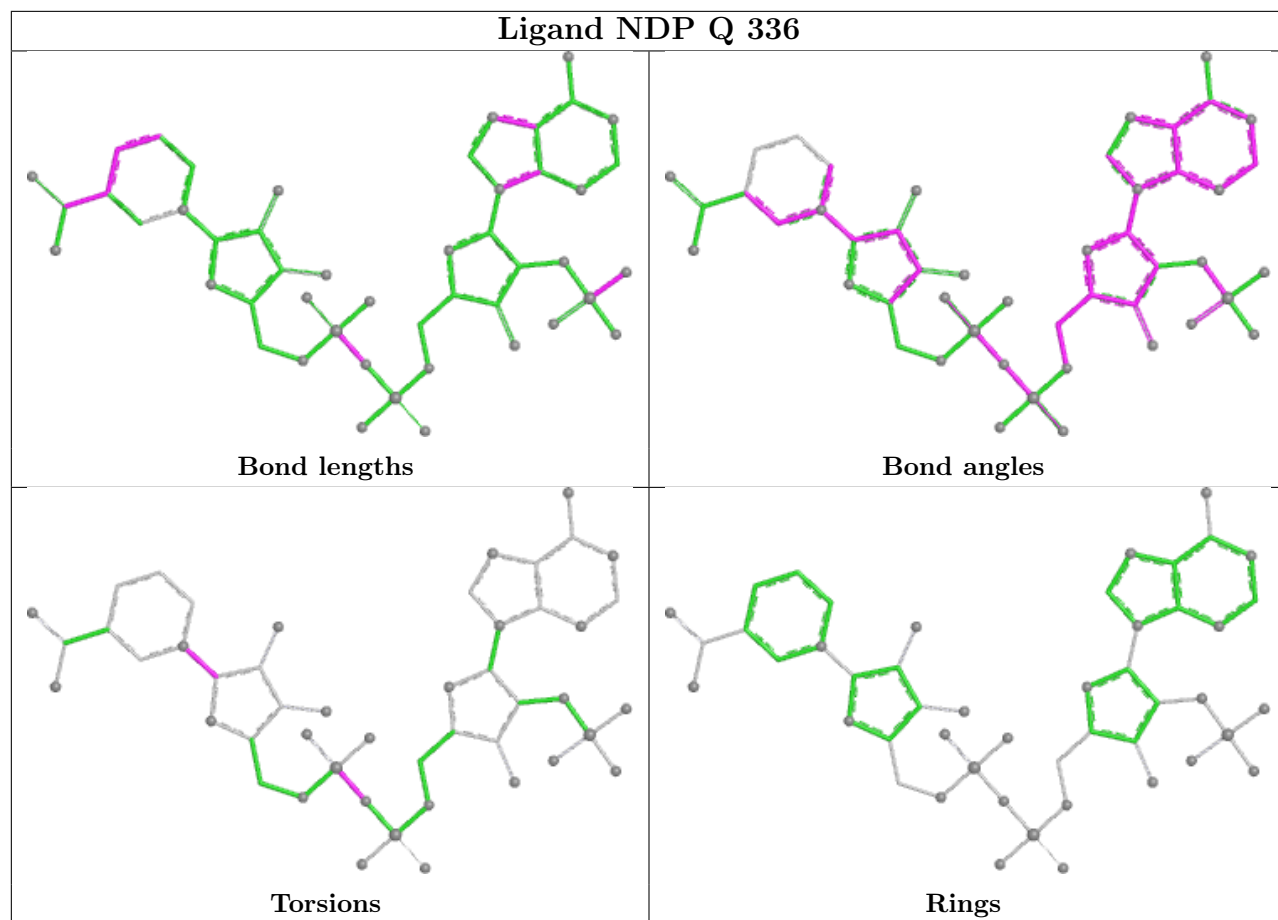
5 monomers are involved in 10 short contacts:

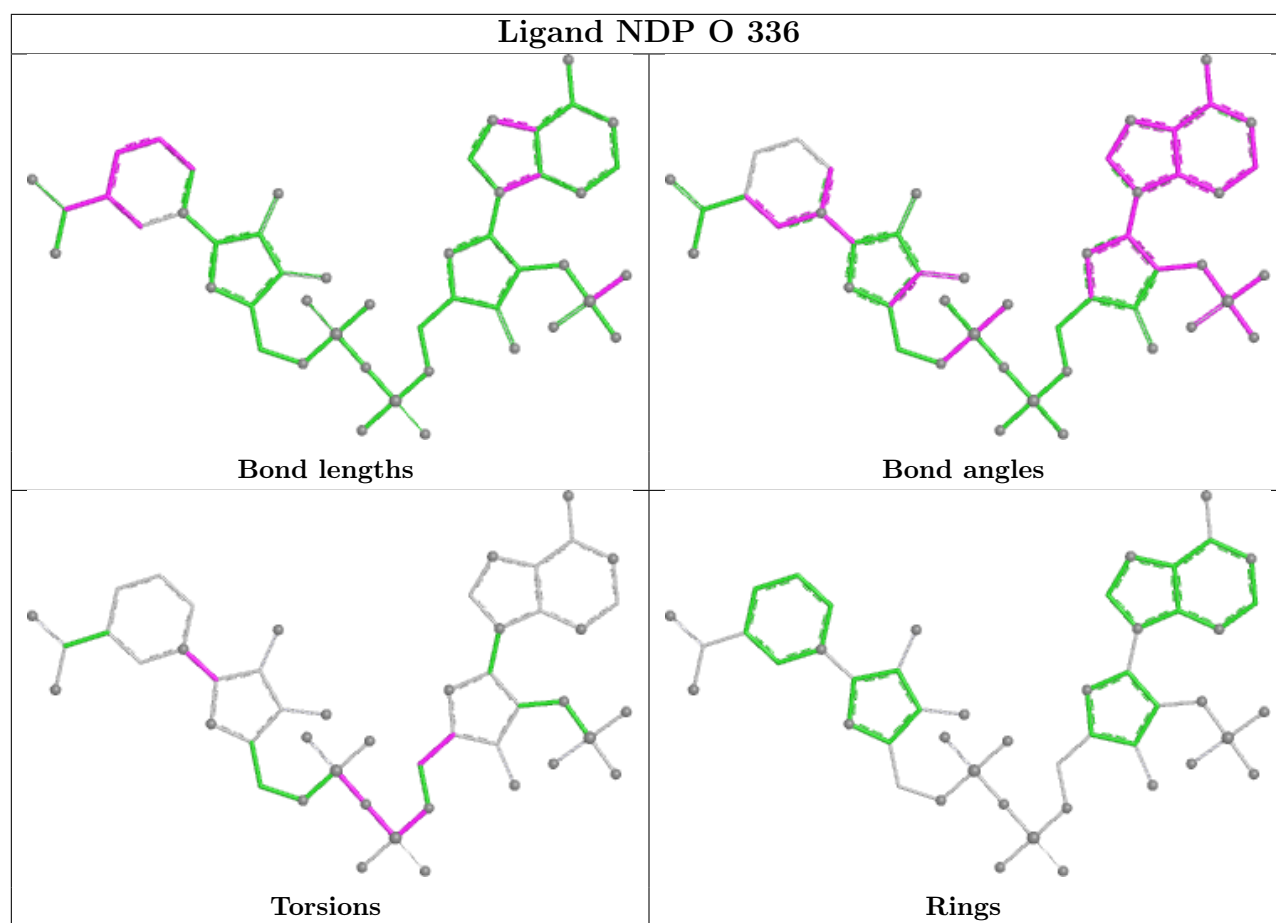
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	336	NDP	2	0
3	P	336	NDP	3	0
3	Q	336	NDP	2	0
2	Q	339	SO4	1	0
3	O	336	NDP	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	O	334/334 (100%)	-1.76	0 100 100	7, 22, 44, 58	0
1	P	334/334 (100%)	-1.76	0 100 100	7, 22, 46, 55	0
1	Q	334/334 (100%)	-1.76	0 100 100	7, 23, 44, 60	0
1	R	334/334 (100%)	-1.76	0 100 100	6, 21, 42, 58	0
All	All	1336/1336 (100%)	-1.76	0 100 100	6, 22, 44, 60	0

There are no RSRZ outliers to report.

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.

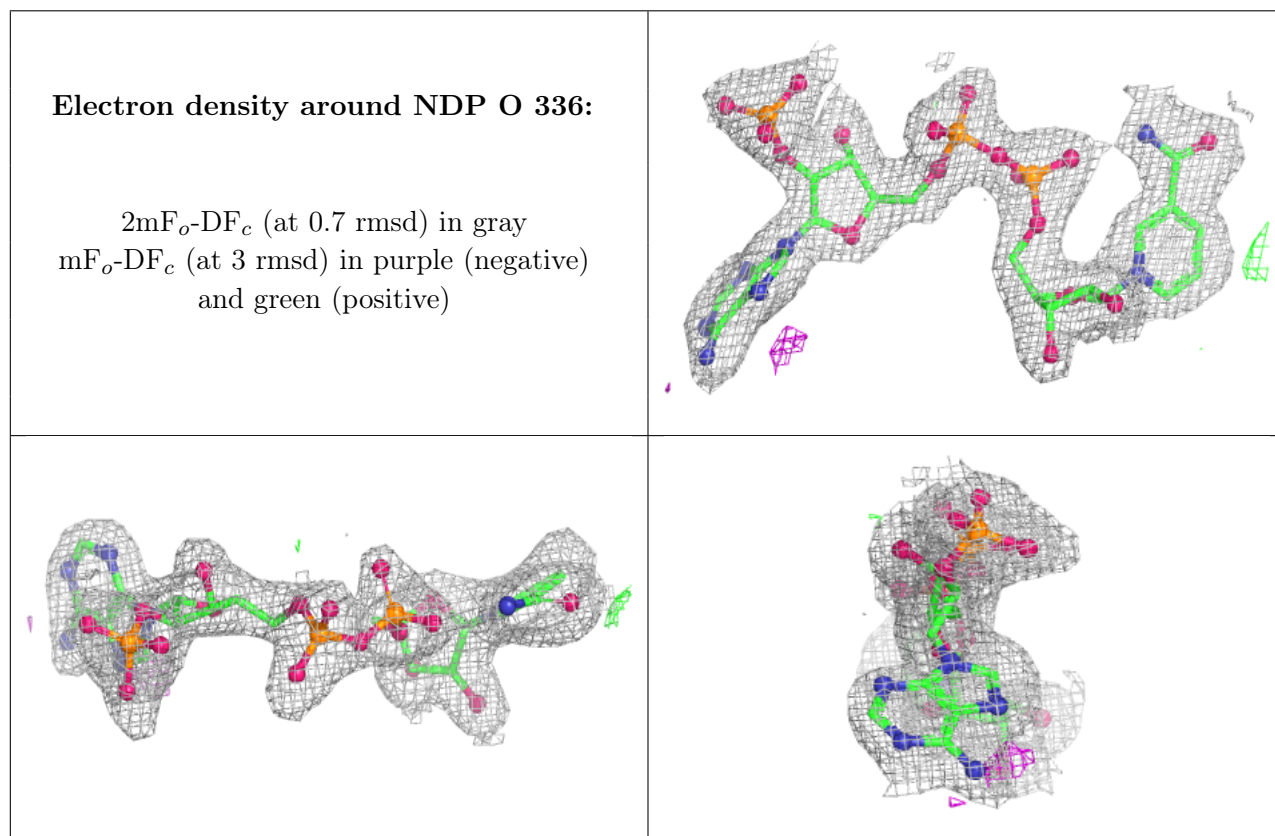
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	O	339	5/5	0.99	0.03	54,56,58,59	0
2	SO4	Q	339	5/5	0.99	0.02	62,63,64,67	0
2	SO4	P	338	5/5	1.00	0.01	40,44,46,47	0
2	SO4	P	339	5/5	1.00	0.02	43,47,49,50	0

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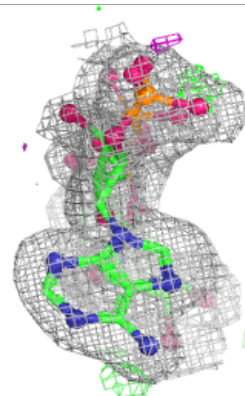
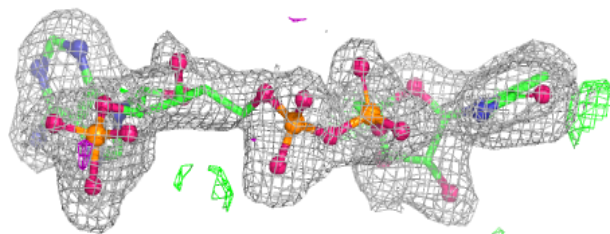
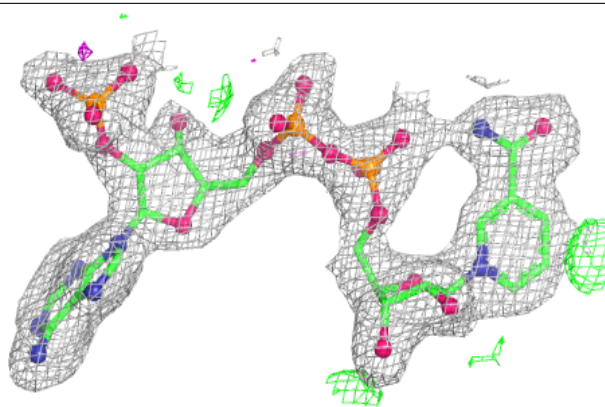
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	Q	338	5/5	1.00	0.01	34,34,38,40	0
2	SO4	O	338	5/5	1.00	0.02	40,40,47,48	0
2	SO4	R	338	5/5	1.00	0.02	49,54,56,56	0
2	SO4	R	339	5/5	1.00	0.03	64,65,67,68	0
3	NDP	O	336	48/48	1.00	0.01	13,22,36,43	0
3	NDP	P	336	48/48	1.00	0.02	10,19,31,34	0
3	NDP	Q	336	48/48	1.00	0.02	6,17,24,29	0
3	NDP	R	336	48/48	1.00	0.02	9,21,30,32	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.

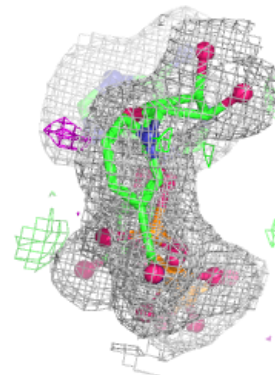
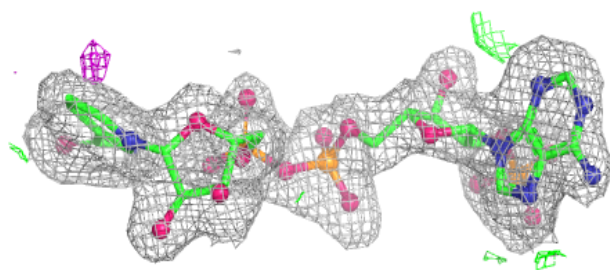
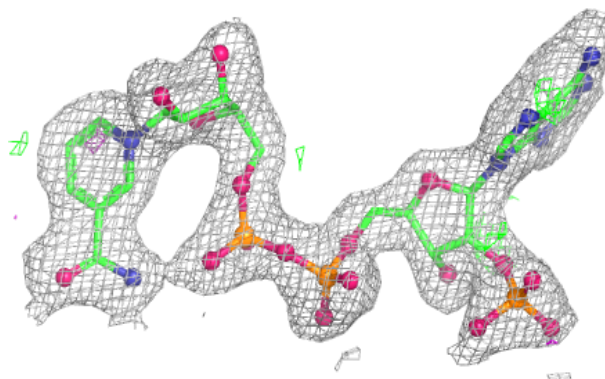


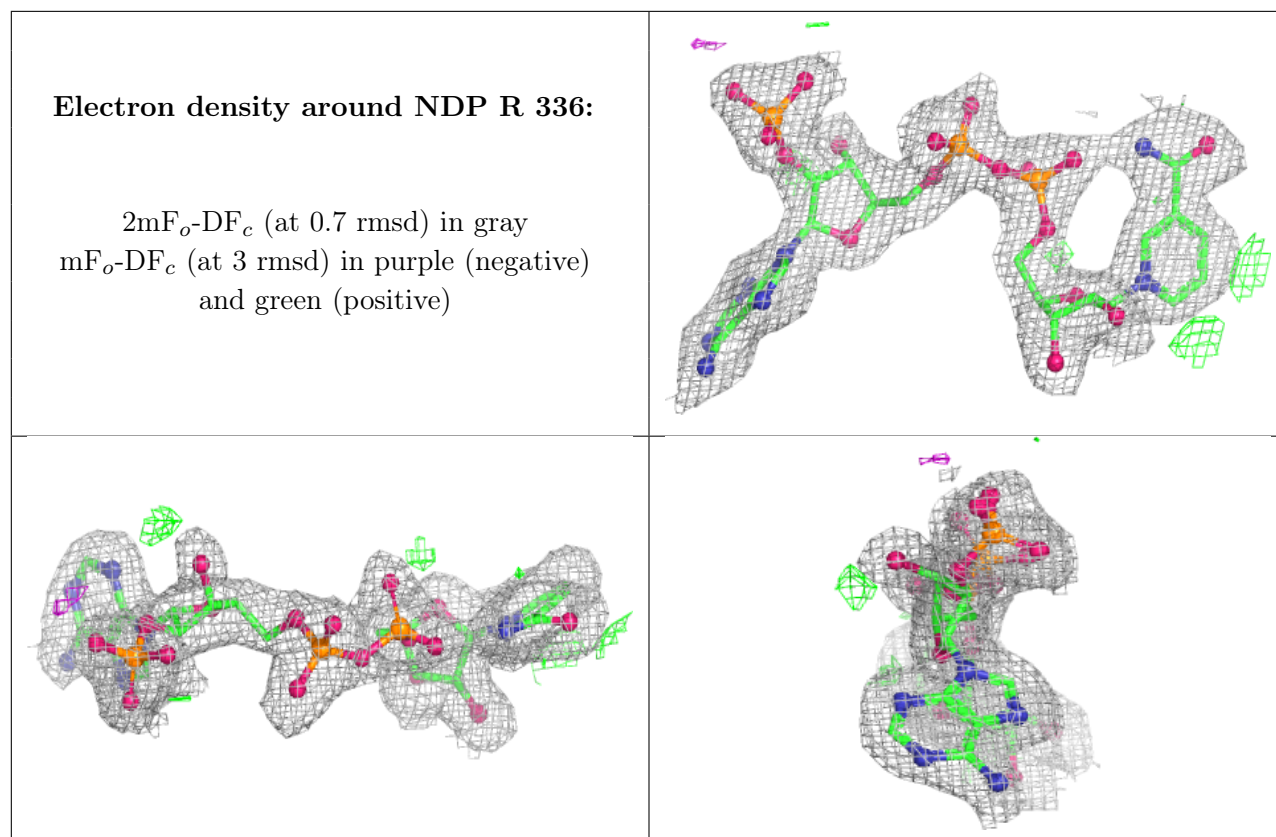
Electron density around NDP P 336:

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

**Electron density around NDP Q 336:**

$2mF_o-DF_c$ (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.