



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:16 AM UTC

PDB ID : 6QUQ / pdb_00006quq
Title : Crystal structure of glutathionylated glycolytic glyceraldehyde-3- phosphate dehydrogenase from Arabidopsis thaliana (AtGAPC1)
Authors : Fermani, S.; Zaffagnini, M.; Falini, G.; Trost, P.
Deposited on : 2019-02-28
Resolution : 2.99 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

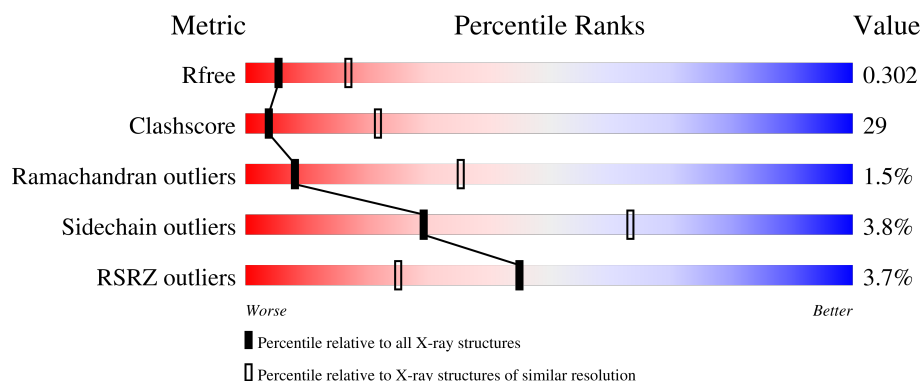
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	
1	R	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	O	403	-	-	X	-
3	SO4	R	403	-	-	X	-
4	GSH	O	404	X	-	X	-
4	GSH	R	404	X	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5325 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 GAPC1, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	333	Total	C	N	O	S	0	0	0
			2559	1627	433	490	9			
1	R	334	Total	C	N	O	S	0	0	0
			2568	1633	435	491	9			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



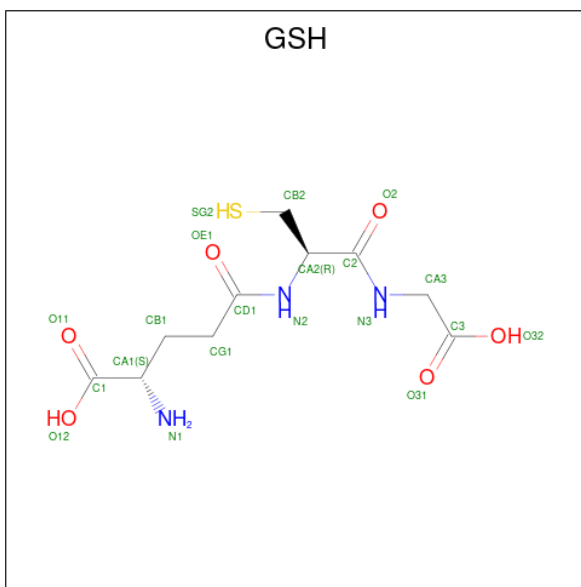
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	O	1	Total 20	C 10	N 3	O 6	S 1	0	0
4	R	1	Total 20	C 10	N 3	O 6	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	18	Total O 18 18	0	0
5	R	17	Total O 17 17	0	0

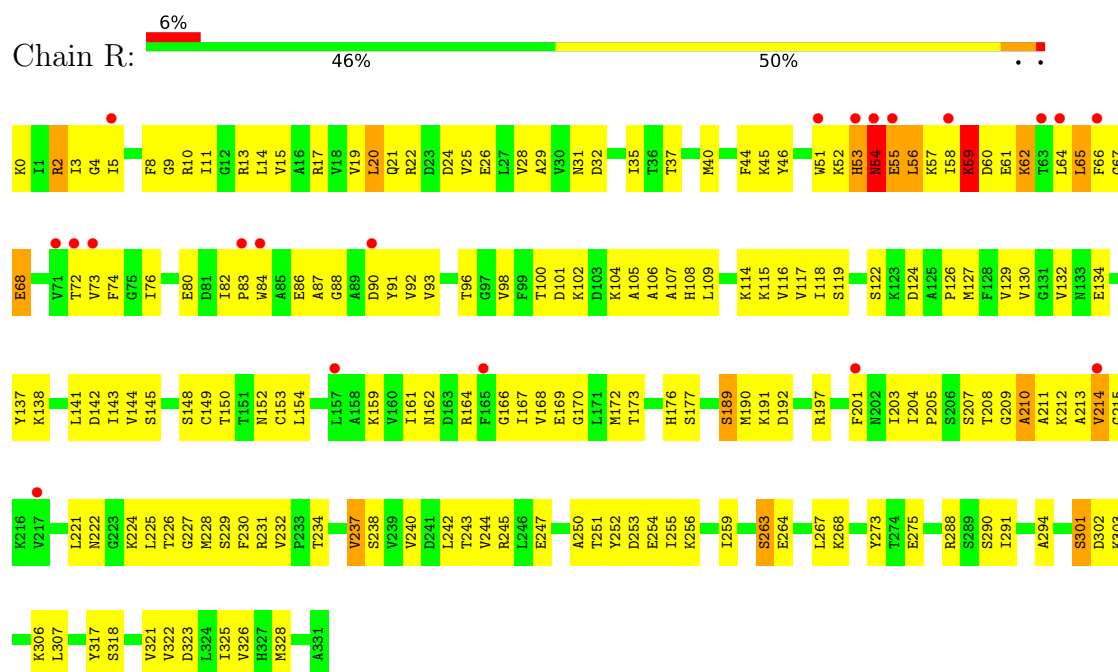
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase GAPC1, cytosolic



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4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.36Å 77.36Å 406.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.66 – 2.99 47.66 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.66-2.99) 99.4 (47.66-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.19 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.249 , 0.303 0.251 , 0.302	Depositor DCC
R_{free} test set	780 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5325	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: SO4, GSH, NAD

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	0.29	0/2607	0.69	2/3528 (0.1%)
1	R	0.44	0/2616	0.82	9/3539 (0.3%)
All	All	0.37	0/5223	0.76	11/7067 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	266	LYS	CG-CD-CE	-7.66	93.69	111.30
1	R	164	ARG	CB-CG-CD	7.21	127.87	111.30
1	R	212	LYS	CA-CB-CG	6.56	127.22	114.10
1	R	68	GLU	CA-CB-CG	-6.49	101.12	114.10
1	R	54	ASN	CB-CA-C	-6.13	107.80	115.89
1	O	266	LYS	CD-CE-NZ	5.70	130.14	111.90
1	R	212	LYS	CG-CD-CE	5.37	123.65	111.30
1	R	68	GLU	N-CA-CB	-5.28	102.51	111.27
1	R	20	LEU	CA-C-N	-5.01	115.12	122.83
1	R	20	LEU	C-N-CA	-5.01	115.12	122.83
1	R	164	ARG	CD-NE-CZ	5.00	131.40	124.40

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	O	2559	0	2582	114	0
1	R	2568	0	2592	183	0
2	O	44	0	26	4	0
2	R	44	0	26	5	0
3	O	15	0	0	3	0
3	R	20	0	0	4	0
4	O	20	0	14	7	0
4	R	20	0	14	14	0
5	O	18	0	0	2	0
5	R	17	0	0	0	0
All	All	5325	0	5254	301	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 29.

All (301) 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:R:208:THR:HB	4:R:404:GSH:N1	1.34	1.38
1:R:208:THR:CB	4:R:404:GSH:HN12	1.43	1.29
1:R:208:THR:OG1	3:R:403:SO4:S	2.06	1.13
1:R:55:GLU:OE2	1:R:66:PHE:HE1	1.33	1.09
1:R:59:LYS:HE2	1:R:59:LYS:HA	1.37	1.06
1:R:55:GLU:OE2	1:R:66:PHE:CE1	2.10	1.05
1:R:2:ARG:CZ	1:R:90:ASP:CG	2.29	1.04
1:R:208:THR:OG1	3:R:403:SO4:O3	1.76	1.01
1:R:82:ILE:HD12	1:R:84:TRP:CE2	1.96	1.00
1:R:2:ARG:NH2	1:R:90:ASP:OD1	1.96	0.99
1:R:208:THR:CG2	4:R:404:GSH:HN12	1.74	0.97
1:R:208:THR:OG1	3:R:403:SO4:O4	1.82	0.95
1:R:208:THR:CB	4:R:404:GSH:N1	2.13	0.94
1:R:102:LYS:HB2	1:R:124:ASP:CG	1.95	0.91
1:R:2:ARG:CZ	1:R:90:ASP:CB	2.41	0.91
1:R:132:VAL:HG23	1:R:159:LYS:HD3	1.54	0.90
1:O:286:ASP:OD1	1:O:288:ARG:HD3	1.72	0.89
1:R:119:SER:O	1:R:317:TYR:OH	1.92	0.87
1:O:132:VAL:HG13	1:O:159:LYS:HD2	1.57	0.85
1:R:82:ILE:HD12	1:R:84:TRP:CZ2	2.12	0.85
1:R:221:LEU:HA	1:R:224:LYS:HD2	1.61	0.83
1:R:2:ARG:NH2	1:R:90:ASP:CG	2.35	0.82
1:R:2:ARG:HB2	1:R:28:VAL:HG21	1.61	0.82
1:R:59:LYS:HA	1:R:59:LYS:CE	2.05	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:208:THR:CG2	4:R:404:GSH:N1	2.42	0.80
1:R:154:LEU:HD11	1:R:242:LEU:HD13	1.61	0.80
1:R:101:ASP:HB2	1:R:104:LYS:HG3	1.64	0.79
1:R:208:THR:HB	4:R:404:GSH:CA1	2.10	0.79
1:R:51:TRP:NE1	1:R:53:HIS:O	2.16	0.79
1:R:138:LYS:H	1:R:141:LEU:CD2	1.94	0.79
1:O:235:VAL:HG22	1:R:201:PHE:CD2	2.18	0.77
1:O:116:VAL:HB	1:O:143:ILE:HG13	1.65	0.77
1:R:138:LYS:H	1:R:141:LEU:HD23	1.50	0.77
1:R:138:LYS:O	1:R:141:LEU:CD2	2.33	0.77
1:R:115:LYS:NZ	1:R:137:TYR:OH	2.19	0.75
1:O:57:LYS:H	1:O:57:LYS:HD2	1.52	0.74
1:O:2:ARG:NH2	5:O:501:HOH:O	2.21	0.74
1:R:213:ALA:C	1:R:215:GLY:H	1.95	0.72
1:O:37:THR:HG21	1:O:61:GLU:O	1.91	0.71
1:O:115:LYS:NZ	1:O:137:TYR:OH	2.23	0.70
1:R:255:ILE:HD11	1:R:307:LEU:HD11	1.75	0.69
1:O:231:ARG:HH21	4:O:404:GSH:HB13	1.58	0.69
1:R:138:LYS:O	1:R:141:LEU:HD22	1.93	0.68
2:R:401:NAD:O2D	4:R:404:GSH:N3	2.22	0.68
1:O:2:ARG:HB3	1:O:28:VAL:HG21	1.76	0.68
1:O:172:MET:HE1	1:O:208:THR:HG21	1.76	0.67
1:R:67:GLY:C	1:R:68:GLU:HG3	2.18	0.67
1:R:148:SER:O	1:R:152:ASN:ND2	2.24	0.67
1:R:54:ASN:HB3	1:R:67:GLY:N	2.09	0.67
1:R:170:GLY:HA3	1:R:244:VAL:HG12	1.77	0.67
1:R:51:TRP:CD1	1:R:53:HIS:O	2.48	0.67
1:O:132:VAL:CG1	1:O:218:LEU:HD11	2.25	0.67
1:O:235:VAL:HG22	1:R:201:PHE:CG	2.29	0.67
1:R:82:ILE:CD1	1:R:84:TRP:CZ2	2.77	0.67
1:R:242:LEU:HD21	1:R:244:VAL:HG13	1.78	0.66
1:O:191:LYS:H	1:O:191:LYS:HD2	1.60	0.66
1:O:22:ARG:NH2	1:O:24:ASP:OD2	2.29	0.66
1:R:24:ASP:OD1	1:R:24:ASP:N	2.28	0.66
1:R:59:LYS:HB3	1:R:62:LYS:HG3	1.76	0.66
1:R:82:ILE:CD1	1:R:84:TRP:CE2	2.77	0.65
1:R:138:LYS:O	1:R:141:LEU:HD23	1.96	0.65
1:O:122:SER:H	1:O:127:MET:HE1	1.62	0.65
1:R:22:ARG:NH2	1:R:24:ASP:OD2	2.18	0.65
1:R:54:ASN:HB3	1:R:67:GLY:H	1.61	0.65
1:O:321:VAL:O	1:O:325:ILE:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:37:THR:HG22	1:R:73:VAL:HG11	1.79	0.64
1:R:229:SER:HB2	4:R:404:GSH:HN11	1.61	0.64
1:R:2:ARG:NE	1:R:90:ASP:CG	2.56	0.64
1:R:5:ILE:HG23	1:R:93:VAL:HB	1.79	0.64
1:O:100:THR:O	1:O:122:SER:OG	2.11	0.64
1:R:96:THR:HG22	1:R:98:VAL:H	1.63	0.64
1:R:154:LEU:HD11	1:R:242:LEU:CD1	2.29	0.63
1:R:149:CYS:SG	1:R:150:THR:N	2.72	0.63
1:O:79:PRO:HB2	1:O:107:ALA:HB3	1.81	0.62
1:O:105:ALA:HB3	1:O:143:ILE:HD11	1.82	0.62
1:O:121:PRO:HD2	4:O:404:GSH:HA32	1.80	0.62
1:R:76:ILE:HB	1:R:82:ILE:HG23	1.79	0.62
1:O:179:THR:OG1	1:O:231:ARG:NH1	2.32	0.62
1:R:83:PRO:HB2	1:R:86:GLU:HG3	1.80	0.62
1:O:28:VAL:O	1:O:71:VAL:HA	2.00	0.61
1:O:132:VAL:HG12	1:O:218:LEU:HD11	1.82	0.61
1:O:54:ASN:O	1:O:66:PHE:HD1	1.84	0.60
1:R:59:LYS:HG3	1:R:62:LYS:HD3	1.81	0.60
1:O:79:PRO:O	1:O:82:ILE:HG13	2.01	0.60
1:O:148:SER:HB2	4:O:404:GSH:HB23	1.84	0.60
1:O:109:LEU:HD21	1:O:142:ASP:HB2	1.83	0.60
1:R:102:LYS:HB2	1:R:124:ASP:OD2	2.02	0.60
1:R:242:LEU:HD21	1:R:244:VAL:CG1	2.32	0.59
1:O:24:ASP:OD1	1:O:24:ASP:N	2.36	0.59
1:R:208:THR:HG21	4:R:404:GSH:HN12	1.65	0.59
1:O:38:GLU:HG3	1:O:57:LYS:HE2	1.84	0.59
1:O:58:ILE:HG23	1:O:63:THR:OG1	2.03	0.59
1:R:2:ARG:HD3	1:R:90:ASP:HB2	1.85	0.59
1:O:41:THR:HG21	1:O:57:LYS:HG3	1.84	0.58
1:O:78:ASN:ND2	1:O:80:GLU:OE2	2.36	0.58
1:O:167:ILE:HD11	1:O:221:LEU:HD13	1.83	0.58
2:O:401:NAD:O2D	4:O:404:GSH:N3	2.35	0.58
1:O:105:ALA:CB	1:O:143:ILE:HD11	2.33	0.58
1:R:2:ARG:CZ	1:R:90:ASP:HB2	2.33	0.58
1:O:102:LYS:HB2	1:O:124:ASP:O	2.03	0.58
1:R:255:ILE:O	1:R:259:ILE:HG13	2.04	0.57
1:R:189:SER:OG	1:R:192:ASP:O	2.21	0.57
3:R:403:SO4:O1	4:R:404:GSH:HA31	2.04	0.57
1:R:243:THR:OG1	1:R:306:LYS:NZ	2.38	0.57
1:O:299:ALA:HA	1:O:305:VAL:HA	1.87	0.57
1:R:9:GLY:O	1:R:13:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:191:LYS:NZ	5:O:504:HOH:O	2.38	0.56
1:O:128:PHE:CE2	1:O:144:VAL:HG21	2.40	0.56
1:R:2:ARG:H	1:R:2:ARG:CD	2.17	0.56
1:R:11:ILE:O	1:R:15:VAL:HG12	2.05	0.56
1:R:318:SER:HA	1:R:321:VAL:HG22	1.88	0.56
1:R:28:VAL:HG21	1:R:88:GLY:O	2.05	0.55
1:O:64:LEU:O	1:O:70:PRO:O	2.25	0.55
1:R:210:ALA:O	1:R:214:VAL:HG23	2.06	0.55
1:O:128:PHE:HE2	1:O:144:VAL:HG21	1.71	0.55
1:R:8:PHE:N	1:R:32:ASP:OD2	2.37	0.55
1:O:41:THR:HG21	1:O:57:LYS:HE3	1.88	0.54
1:R:142:ASP:N	1:R:142:ASP:OD1	2.35	0.54
3:O:403:SO4:O3	4:O:404:GSH:HG13	2.07	0.54
1:O:41:THR:HG21	1:O:57:LYS:CE	2.37	0.53
1:O:144:VAL:HG22	1:O:145:SER:H	1.73	0.53
2:R:401:NAD:O1N	2:R:401:NAD:N7N	2.40	0.53
1:O:206:SER:OG	1:O:207:SER:N	2.42	0.53
1:R:54:ASN:N	1:R:54:ASN:HD22	2.05	0.53
1:O:57:LYS:HD2	1:O:57:LYS:N	2.21	0.53
1:R:19:VAL:HA	1:R:25:VAL:HG21	1.91	0.53
1:O:324:LEU:O	1:O:328:MET:HG3	2.10	0.52
1:R:208:THR:HB	4:R:404:GSH:HA1	1.91	0.52
1:O:236:ASP:OD1	1:O:237:VAL:N	2.40	0.52
1:R:59:LYS:CE	1:R:59:LYS:CA	2.85	0.52
1:R:242:LEU:CD2	1:R:244:VAL:HG13	2.39	0.52
1:O:114:LYS:O	1:O:115:LYS:HD3	2.10	0.51
1:O:159:LYS:O	1:O:163:ASP:HB2	2.09	0.51
1:O:15:VAL:HG23	1:O:318:SER:HB3	1.92	0.51
1:O:18:VAL:O	1:O:22:ARG:HG2	2.10	0.51
1:R:91:TYR:HB3	1:R:325:ILE:HD13	1.93	0.51
1:O:41:THR:CB	1:O:57:LYS:HE3	2.41	0.51
1:O:74:PHE:HB3	1:O:76:ILE:HD13	1.92	0.51
1:R:124:ASP:OD1	1:R:124:ASP:N	2.43	0.51
1:R:170:GLY:CA	1:R:244:VAL:HG12	2.40	0.51
1:R:213:ALA:C	1:R:215:GLY:N	2.64	0.51
1:R:154:LEU:HD13	1:R:240:VAL:HG11	1.92	0.51
1:O:9:GLY:O	1:O:13:ARG:HG3	2.11	0.51
1:O:255:ILE:O	1:O:259:ILE:HG13	2.10	0.51
1:O:80:GLU:N	1:O:107:ALA:HB1	2.26	0.50
1:R:100:THR:O	1:R:122:SER:OG	2.25	0.50
1:O:326:VAL:O	1:O:329:SER:OG	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:ILE:HB	1:R:26:GLU:O	2.12	0.50
1:R:100:THR:O	1:R:118:ILE:HD13	2.12	0.50
1:R:109:LEU:HD11	1:R:143:ILE:HD11	1.94	0.50
1:R:54:ASN:N	1:R:54:ASN:ND2	2.60	0.50
1:R:137:TYR:CZ	1:R:328:MET:HB3	2.46	0.50
1:R:214:VAL:HG12	1:R:214:VAL:O	2.12	0.50
1:R:56:LEU:O	1:R:65:LEU:N	2.32	0.49
1:O:326:VAL:O	1:O:330:LYS:HG2	2.11	0.49
1:O:130:VAL:HA	1:O:134:GLU:HB3	1.93	0.49
1:R:21:GLN:NE2	1:R:53:HIS:CD2	2.81	0.49
1:R:76:ILE:HB	1:R:82:ILE:CG2	2.42	0.49
1:R:142:ASP:C	1:R:143:ILE:HG13	2.38	0.49
1:R:106:ALA:HA	1:R:143:ILE:HD11	1.95	0.49
1:O:200:SER:HA	1:O:233:PRO:HB3	1.94	0.49
1:O:15:VAL:CG2	1:O:318:SER:HB3	2.42	0.49
1:O:217:VAL:O	1:O:218:LEU:HD12	2.13	0.49
1:O:170:GLY:HA3	1:O:225:LEU:HD23	1.95	0.48
1:R:9:GLY:HA3	2:R:401:NAD:O5B	2.14	0.48
1:O:208:THR:OG1	3:O:403:SO4:O3	2.32	0.48
1:O:176:HIS:HA	1:O:238:SER:HB3	1.95	0.48
1:R:4:GLY:HA2	1:R:29:ALA:O	2.13	0.48
1:R:20:LEU:HD11	1:R:66:PHE:CD2	2.49	0.48
1:R:22:ARG:HB2	1:R:25:VAL:HG22	1.96	0.48
1:R:224:LYS:O	1:R:225:LEU:HD23	2.14	0.48
1:O:83:PRO:HB2	1:O:86:GLU:HB2	1.96	0.48
1:R:162:ASN:CG	1:R:221:LEU:HD21	2.38	0.48
1:R:203:ILE:HG23	1:R:232:VAL:HG12	1.95	0.48
1:R:102:LYS:CB	1:R:124:ASP:OD2	2.61	0.48
1:O:6:ASN:OD1	1:O:31:ASN:ND2	2.42	0.47
1:O:80:GLU:HA	1:O:107:ALA:O	2.14	0.47
1:O:217:VAL:HG23	1:O:218:LEU:HD13	1.95	0.47
1:O:299:ALA:HB2	1:O:305:VAL:HG23	1.96	0.47
1:O:317:TYR:O	1:O:321:VAL:HG23	2.14	0.47
1:O:57:LYS:H	1:O:57:LYS:CD	2.24	0.47
1:R:215:GLY:HA3	1:R:222:ASN:HA	1.96	0.47
1:R:4:GLY:O	1:R:92:VAL:HA	2.14	0.47
1:R:322:VAL:O	1:R:326:VAL:HG13	2.15	0.47
1:R:84:TRP:O	1:R:87:ALA:O	2.33	0.47
2:R:401:NAD:HO2N	4:R:404:GSH:HN3	1.57	0.47
1:O:14:LEU:O	1:O:18:VAL:HG23	2.15	0.47
1:R:251:THR:OG1	1:R:254:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:101:ASP:HA	1:R:122:SER:OG	2.15	0.46
1:R:80:GLU:CG	1:R:107:ALA:HB1	2.46	0.46
1:O:123:LYS:HA	1:O:123:LYS:HD3	1.63	0.46
1:O:35:ILE:HG12	1:O:43:MET:HE1	1.97	0.46
1:R:229:SER:OG	4:R:404:GSH:O11	2.28	0.46
1:R:213:ALA:O	1:R:215:GLY:N	2.49	0.46
1:R:273:TYR:OH	1:R:275:GLU:OE2	2.25	0.46
1:R:44:PHE:HE2	1:R:51:TRP:CD1	2.34	0.46
1:R:176:HIS:HA	1:R:238:SER:HB3	1.97	0.46
1:O:9:GLY:HA3	2:O:401:NAD:O5B	2.16	0.46
1:O:32:ASP:OD2	2:O:401:NAD:H1B	2.15	0.46
1:R:2:ARG:HB2	1:R:28:VAL:CG2	2.38	0.46
1:R:80:GLU:HG2	1:R:107:ALA:O	2.15	0.46
1:R:32:ASP:CG	1:R:35:ILE:HD12	2.41	0.46
1:O:118:ILE:N	1:O:144:VAL:O	2.47	0.45
1:O:322:VAL:HA	1:O:325:ILE:HG13	1.97	0.45
1:O:95:SER:HA	1:O:119:SER:HB3	1.98	0.45
1:O:134:GLU:OE1	1:O:134:GLU:N	2.47	0.45
1:R:130:VAL:HA	1:R:134:GLU:HB3	1.98	0.45
1:R:189:SER:OG	1:R:189:SER:O	2.35	0.45
1:R:2:ARG:CD	1:R:90:ASP:HB2	2.45	0.45
1:R:31:ASN:HA	1:R:74:PHE:O	2.17	0.45
1:R:117:VAL:HG21	1:R:325:ILE:HG12	1.98	0.45
1:O:8:PHE:CG	1:O:13:ARG:HG2	2.51	0.45
1:O:182:GLN:OE1	1:O:231:ARG:HD2	2.17	0.45
1:R:2:ARG:HD3	1:R:2:ARG:H	1.82	0.45
1:R:117:VAL:HA	1:R:144:VAL:HG12	1.98	0.44
1:R:153:CYS:HA	1:R:290:SER:HB2	1.99	0.44
1:O:46:TYR:HB3	1:R:197:ARG:HH12	1.83	0.44
1:O:144:VAL:HG22	1:O:145:SER:N	2.32	0.44
1:O:209:GLY:N	3:O:403:SO4:O2	2.46	0.44
1:R:288:ARG:HB2	1:R:291:ILE:HD11	2.00	0.44
1:O:2:ARG:HD3	1:O:88:GLY:O	2.17	0.44
2:O:401:NAD:C5N	4:O:404:GSH:HB22	2.47	0.44
1:R:127:MET:HE3	1:R:127:MET:HB2	1.87	0.44
1:R:172:MET:HE2	1:R:227:GLY:HA3	1.98	0.44
1:R:32:ASP:OD2	2:R:401:NAD:H1B	2.18	0.44
1:R:13:ARG:O	1:R:17:ARG:HG3	2.18	0.44
1:R:126:PRO:O	1:R:145:SER:N	2.47	0.44
1:R:209:GLY:O	1:R:211:ALA:N	2.50	0.44
1:O:55:GLU:HA	1:O:65:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:45:LYS:HE2	1:R:46:TYR:CZ	2.53	0.43
1:R:10:ARG:HD2	1:R:10:ARG:HA	1.72	0.43
1:R:204:ILE:HB	1:R:231:ARG:HB2	2.00	0.43
1:R:250:ALA:O	1:R:302:ASP:HB3	2.18	0.43
1:R:90:ASP:OD1	1:R:114:LYS:HB2	2.18	0.43
1:O:58:ILE:HB	1:O:65:LEU:CD1	2.48	0.43
1:O:148:SER:N	1:O:151:THR:OG1	2.49	0.43
1:R:83:PRO:HB2	1:R:86:GLU:CG	2.46	0.43
1:R:149:CYS:H	4:R:404:GSH:HB22	1.83	0.43
1:R:173:THR:HG23	1:R:228:MET:HG3	1.99	0.43
1:O:132:VAL:HG11	1:O:218:LEU:HD11	1.98	0.43
1:O:236:ASP:O	1:O:237:VAL:HB	2.18	0.43
1:R:102:LYS:HB2	1:R:124:ASP:OD1	2.17	0.43
1:R:323:ASP:O	1:R:326:VAL:HG22	2.18	0.43
1:O:94:GLU:OE1	1:O:96:THR:OG1	2.23	0.43
1:R:14:LEU:HD23	1:R:17:ARG:HD2	2.00	0.43
1:R:108:HIS:HD2	1:R:116:VAL:HG21	1.82	0.43
1:R:154:LEU:HD12	1:R:154:LEU:HA	1.72	0.43
1:O:289:SER:OG	1:O:320:ARG:HD2	2.19	0.43
1:O:41:THR:OG1	1:O:57:LYS:HE3	2.18	0.42
1:R:3:ILE:H	1:R:28:VAL:HG23	1.84	0.42
1:R:167:ILE:HD12	1:R:221:LEU:HD11	2.01	0.42
1:R:211:ALA:HB3	1:R:226:THR:HA	2.01	0.42
1:O:8:PHE:CD2	1:O:13:ARG:HG2	2.54	0.42
1:O:220:ALA:O	1:O:224:LYS:NZ	2.52	0.42
1:O:253:ASP:HA	1:O:256:LYS:HD3	2.01	0.42
1:R:22:ARG:HB2	1:R:25:VAL:CG2	2.48	0.42
1:O:159:LYS:HB2	1:O:218:LEU:HD21	2.00	0.42
1:R:53:HIS:ND1	1:R:53:HIS:N	2.67	0.42
1:R:15:VAL:HB	1:R:318:SER:HB3	2.00	0.42
1:R:253:ASP:HA	1:R:256:LYS:HD3	2.02	0.42
1:O:79:PRO:HB2	1:O:107:ALA:CB	2.50	0.42
1:O:121:PRO:HD2	4:O:404:GSH:CA3	2.49	0.42
1:R:177:SER:HB3	1:R:234:THR:O	2.20	0.42
1:O:19:VAL:CG1	1:O:322:VAL:HG11	2.50	0.42
1:O:41:THR:CG2	1:O:57:LYS:HE3	2.50	0.42
1:R:161:ILE:HD12	1:R:255:ILE:HD11	2.01	0.42
1:R:168:VAL:HG23	1:R:169:GLU:N	2.34	0.42
1:R:80:GLU:H	1:R:80:GLU:HG3	1.46	0.42
1:R:167:ILE:HG23	1:R:244:VAL:HB	2.01	0.42
1:R:245:ARG:HA	1:R:303:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:263:SER:O	1:R:268:LYS:HA	2.20	0.42
1:O:122:SER:H	1:O:127:MET:CE	2.31	0.42
1:R:35:ILE:HG22	1:R:40:MET:HG3	2.02	0.41
1:R:114:LYS:C	1:R:115:LYS:HG2	2.45	0.41
1:R:267:LEU:HA	1:R:267:LEU:HD23	1.78	0.41
1:O:41:THR:HG21	1:O:57:LYS:CG	2.49	0.41
1:R:29:ALA:HA	1:R:72:THR:O	2.20	0.41
1:R:191:LYS:N	1:R:191:LYS:HD3	2.35	0.41
1:R:205:PRO:HG3	1:R:230:PHE:HE1	1.84	0.41
1:O:8:PHE:CE1	1:O:13:ARG:HA	2.55	0.41
1:O:58:ILE:CG2	1:O:63:THR:OG1	2.67	0.41
1:R:247:GLU:H	1:R:247:GLU:HG2	1.68	0.41
1:R:17:ARG:HG2	1:R:44:PHE:CE1	2.56	0.41
1:R:96:THR:CG2	1:R:98:VAL:HG22	2.51	0.41
1:R:177:SER:OG	1:R:237:VAL:O	2.34	0.41
1:O:58:ILE:HB	1:O:65:LEU:HD11	2.02	0.41
1:O:106:ALA:HA	1:O:109:LEU:HD12	2.02	0.41
1:R:105:ALA:HB2	1:R:118:ILE:HD11	2.01	0.41
1:R:116:VAL:HG12	1:R:143:ILE:HG12	2.03	0.41
1:O:272:GLY:HA3	1:O:288:ARG:HH21	1.85	0.41
1:O:260:LYS:O	1:O:263:SER:OG	2.21	0.41
1:R:62:LYS:HB2	1:R:62:LYS:HE2	1.37	0.40
1:R:162:ASN:O	1:R:166:GLY:N	2.51	0.40
1:R:172:MET:HG2	1:R:173:THR:N	2.36	0.40
1:O:127:MET:HG2	1:O:147:ALA:HB2	2.04	0.40
1:O:170:GLY:O	1:O:225:LEU:HA	2.21	0.40
1:R:154:LEU:HD22	1:R:172:MET:SD	2.61	0.40
1:R:190:MET:HB3	1:R:191:LYS:HD3	2.03	0.40
1:R:252:TYR:OH	1:R:294:ALA:O	2.23	0.40
1:R:129:VAL:HB	1:R:132:VAL:CG1	2.52	0.40
1:R:301:SER:HB3	1:R:303:LYS:H	1.86	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	O	331/334 (99%)	313 (95%)	12 (4%)	6 (2%)	6	31
1	R	332/334 (99%)	308 (93%)	20 (6%)	4 (1%)	10	40
All	All	663/668 (99%)	621 (94%)	32 (5%)	10 (2%)	8	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	70	PRO
1	R	214	VAL
1	O	237	VAL
1	R	210	ALA
1	R	237	VAL
1	O	119	SER
1	R	59	LYS
1	O	71	VAL
1	O	330	LYS
1	O	166	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	278/279 (100%)	277 (100%)	1 (0%)	84	90
1	R	279/279 (100%)	259 (93%)	20 (7%)	13	43
All	All	557/558 (100%)	536 (96%)	21 (4%)	29	63

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	57	LYS
1	R	0	LYS
1	R	2	ARG

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Mol	Chain	Res	Type
1	R	52	LYS
1	R	53	HIS
1	R	54	ASN
1	R	55	GLU
1	R	56	LEU
1	R	57	LYS
1	R	58	ILE
1	R	59	LYS
1	R	60	ASP
1	R	61	GLU
1	R	62	LYS
1	R	64	LEU
1	R	65	LEU
1	R	189	SER
1	R	207	SER
1	R	263	SER
1	R	264	GLU
1	R	301	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	21	GLN
1	R	54	ASN
1	R	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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	SO4	O	405	-	4,4,4	0.23	0	6,6,6	0.07	0
2	NAD	R	401	-	46,48,48	1.72	5 (10%)	64,73,73	1.53	8 (12%)
3	SO4	R	402	-	4,4,4	0.23	0	6,6,6	0.05	0
3	SO4	O	402	-	4,4,4	0.24	0	6,6,6	0.09	0
4	GSH	R	404	1	18,19,19	3.20	2 (11%)	21,24,24	1.49	5 (23%)
2	NAD	O	401	-	46,48,48	1.71	5 (10%)	64,73,73	1.61	8 (12%)
3	SO4	O	403	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	R	405	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	R	406	-	4,4,4	0.24	0	6,6,6	0.08	0
4	GSH	O	404	1	18,19,19	3.13	2 (11%)	21,24,24	2.05	5 (23%)
3	SO4	R	403	-	4,4,4	0.19	0	6,6,6	0.36	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
2	NAD	R	401	-	-	7/30/62/62	0/5/5/5
4	GSH	O	404	1	1/1/6/8	12/24/24/24	-
2	NAD	O	401	-	-	7/30/62/62	0/5/5/5
4	GSH	R	404	1	1/1/6/8	13/24/24/24	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	404	GSH	O2-C2	9.44	1.41	1.23
4	R	404	GSH	O2-C2	9.42	1.41	1.23
2	O	401	NAD	O7N-C7N	9.31	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	401	NAD	O7N-C7N	9.26	1.41	1.24
4	R	404	GSH	OE1-CD1	9.14	1.41	1.23
4	O	404	GSH	OE1-CD1	8.63	1.40	1.23
2	R	401	NAD	C2A-N1A	2.54	1.38	1.33
2	O	401	NAD	C2A-N1A	2.53	1.38	1.33
2	R	401	NAD	C2A-N3A	2.51	1.38	1.33
2	O	401	NAD	C2A-N3A	2.50	1.38	1.33
2	O	401	NAD	C8A-N7A	2.25	1.36	1.31
2	R	401	NAD	C2N-N1N	2.23	1.37	1.35
2	R	401	NAD	C8A-N7A	2.09	1.35	1.31
2	O	401	NAD	C2N-N1N	2.02	1.37	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	404	GSH	CG1-CB1-CA1	-6.32	99.37	113.86
2	O	401	NAD	N3A-C2A-N1A	-5.83	119.76	128.58
2	R	401	NAD	N3A-C2A-N1A	-5.77	119.85	128.58
2	O	401	NAD	C5A-C4A-N3A	-4.43	120.61	126.72
2	R	401	NAD	C5A-C4A-N3A	-4.27	120.83	126.72
2	R	401	NAD	N9A-C8A-N7A	-4.14	108.06	113.94
2	O	401	NAD	N9A-C8A-N7A	-4.14	108.06	113.94
4	R	404	GSH	CB1-CG1-CD1	-3.87	104.43	113.06
2	O	401	NAD	C2A-N3A-C4A	3.53	120.45	111.83
2	O	401	NAD	C5A-N7A-C8A	3.53	108.99	103.45
2	R	401	NAD	C2A-N3A-C4A	3.45	120.25	111.83
2	R	401	NAD	C5A-N7A-C8A	3.39	108.78	103.45
4	O	404	GSH	CB2-CA2-N2	-3.21	106.70	111.28
4	O	404	GSH	CB1-CA1-C1	-3.12	102.19	110.45
2	R	401	NAD	N3A-C4A-N9A	2.96	132.21	127.17
2	O	401	NAD	N3A-C4A-N9A	2.83	131.98	127.17
4	O	404	GSH	CA2-CB2-SG2	-2.54	111.30	114.16
2	O	401	NAD	C4A-C5A-N7A	-2.50	107.73	110.58
4	O	404	GSH	O12-C1-O11	-2.47	118.48	124.08
2	R	401	NAD	C4A-N9A-C8A	2.36	108.22	105.74
2	O	401	NAD	O4B-C1B-N9A	2.32	112.54	108.09
2	R	401	NAD	C4A-C5A-N7A	-2.26	107.99	110.58
4	R	404	GSH	CB1-CA1-C1	-2.23	104.55	110.45
4	R	404	GSH	CB2-CA2-N2	-2.18	108.18	111.28
4	R	404	GSH	O32-C3-CA3	2.17	121.05	112.81
4	R	404	GSH	CA2-CB2-SG2	-2.14	111.74	114.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	O	404	GSH	CA1
4	R	404	GSH	CA1

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	401	NAD	O4D-C1D-N1N-C2N
2	O	401	NAD	O4D-C1D-N1N-C6N
2	O	401	NAD	C2D-C1D-N1N-C2N
2	O	401	NAD	C2D-C1D-N1N-C6N
2	R	401	NAD	O4D-C1D-N1N-C2N
2	R	401	NAD	O4D-C1D-N1N-C6N
2	R	401	NAD	C2D-C1D-N1N-C2N
2	R	401	NAD	C2D-C1D-N1N-C6N
4	O	404	GSH	N1-CA1-CB1-CG1
4	O	404	GSH	C1-CA1-CB1-CG1
4	O	404	GSH	CA2-C2-N3-CA3
4	O	404	GSH	O2-C2-N3-CA3
4	R	404	GSH	N1-CA1-CB1-CG1
4	R	404	GSH	C1-CA1-CB1-CG1
4	R	404	GSH	C2-CA2-CB2-SG2
4	R	404	GSH	CA2-C2-N3-CA3
4	R	404	GSH	O2-C2-N3-CA3
4	O	404	GSH	O31-C3-CA3-N3
4	O	404	GSH	O32-C3-CA3-N3
2	O	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	C3B-C4B-C5B-O5B
2	R	401	NAD	O4B-C4B-C5B-O5B
4	O	404	GSH	C2-CA2-CB2-SG2
4	R	404	GSH	O31-C3-CA3-N3
4	R	404	GSH	O32-C3-CA3-N3
2	R	401	NAD	C3B-C4B-C5B-O5B
4	R	404	GSH	O12-C1-CA1-N1
4	O	404	GSH	OE1-CD1-N2-CA2
4	R	404	GSH	O11-C1-CA1-N1
2	R	401	NAD	C2B-C1B-N9A-C8A
4	O	404	GSH	O2-C2-CA2-CB2
4	O	404	GSH	CG1-CD1-N2-CA2
4	R	404	GSH	OE1-CD1-N2-CA2
4	O	404	GSH	O12-C1-CA1-N1
4	R	404	GSH	C3-CA3-N3-C2
2	O	401	NAD	C2B-C1B-N9A-C8A

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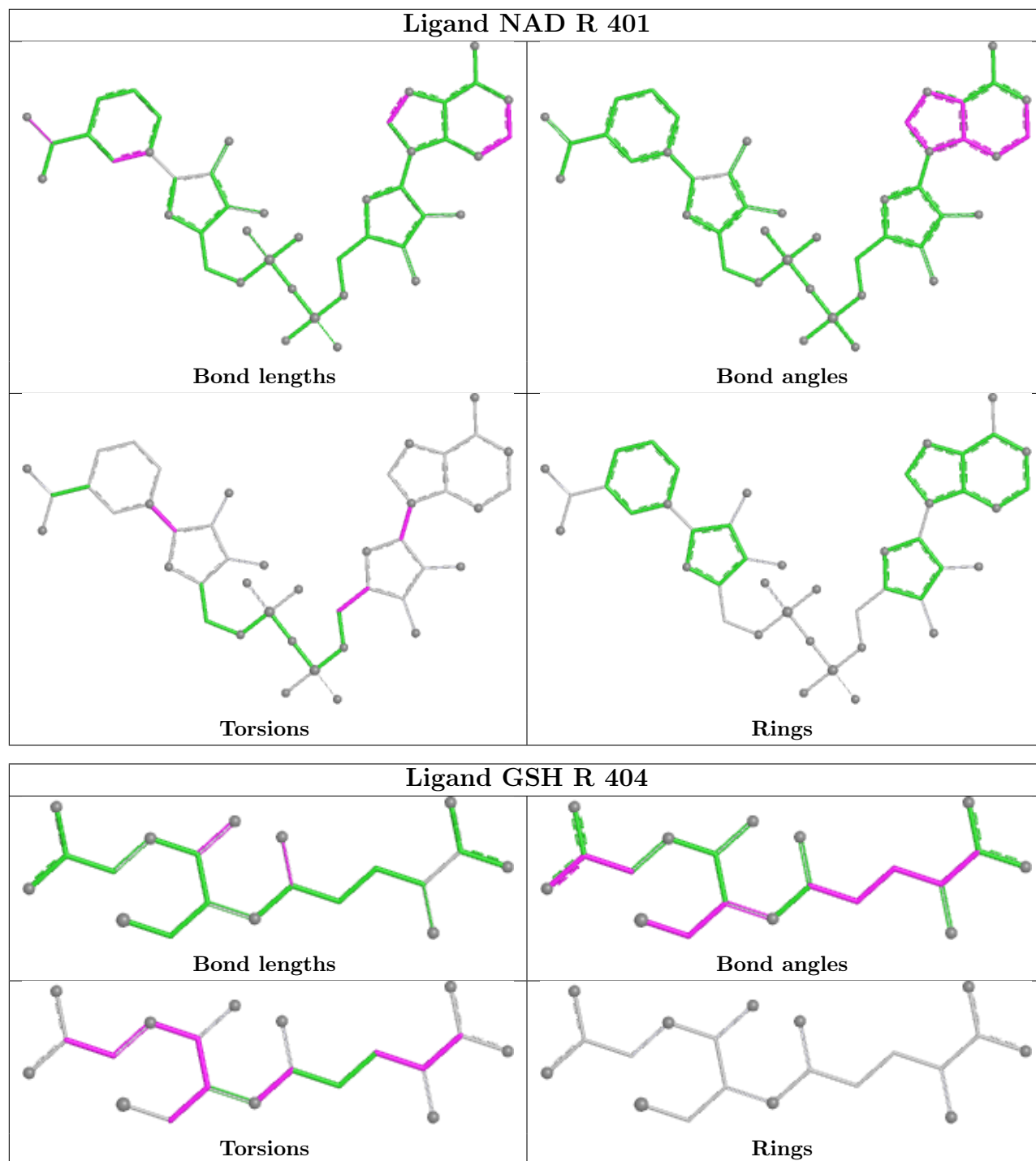
Mol	Chain	Res	Type	Atoms
4	R	404	GSH	O2-C2-CA2-CB2
4	O	404	GSH	O11-C1-CA1-N1
4	R	404	GSH	O2-C2-CA2-N2

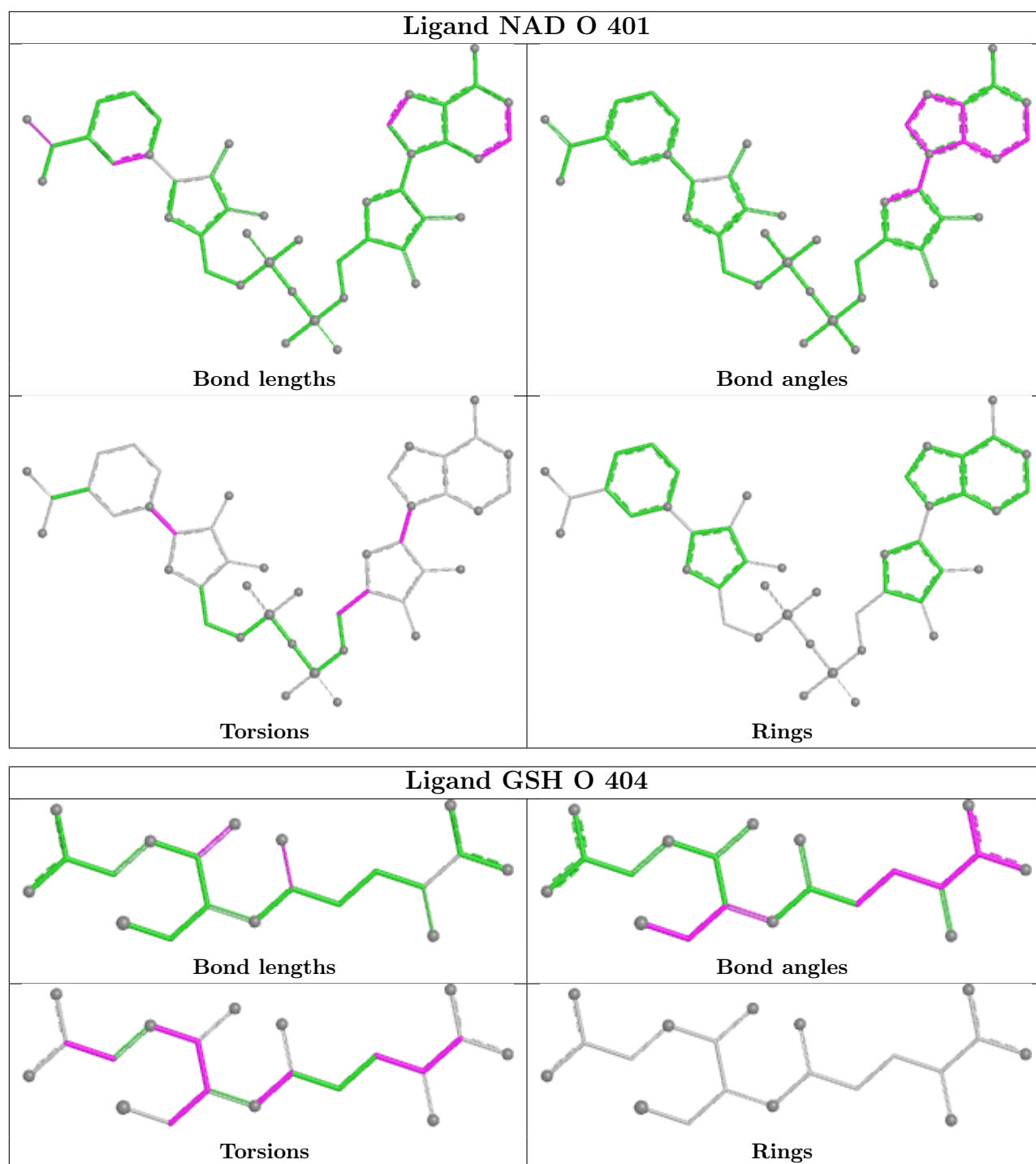
There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	401	NAD	5	0
4	R	404	GSH	14	0
2	O	401	NAD	4	0
3	O	403	SO4	3	0
4	O	404	GSH	7	0
3	R	403	SO4	4	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	O	333/334 (99%)	0.20	5 (1%)	72	49	34, 64, 107, 146	0
1	R	334/334 (100%)	0.53	20 (5%)	27	14	34, 76, 124, 182	0
All	All	667/668 (99%)	0.37	25 (3%)	45	25	34, 71, 115, 182	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	73	VAL	5.3
1	R	64	LEU	5.0
1	R	90	ASP	3.4
1	R	63	THR	3.3
1	R	214	VAL	3.3
1	R	217	VAL	3.1
1	R	201	PHE	2.9
1	O	125	ALA	2.8
1	R	54	ASN	2.8
1	R	72	THR	2.8
1	R	71	VAL	2.7
1	R	66	PHE	2.5
1	O	27	LEU	2.4
1	R	51	TRP	2.4
1	R	58	ILE	2.4
1	R	55	GLU	2.3
1	R	53	HIS	2.3
1	O	126	PRO	2.3
1	R	157	LEU	2.2
1	R	5	ILE	2.2
1	O	142	ASP	2.2
1	R	83	PRO	2.2
1	R	84	TRP	2.1
1	O	29	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	165	PHE	2.1

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](#)

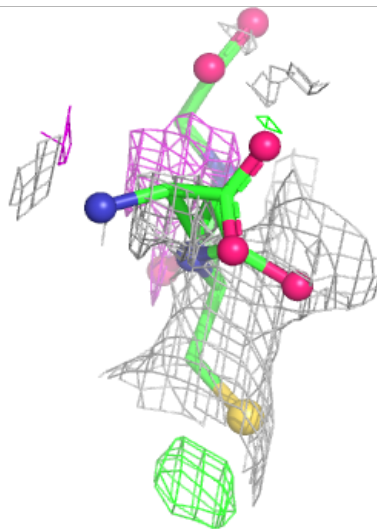
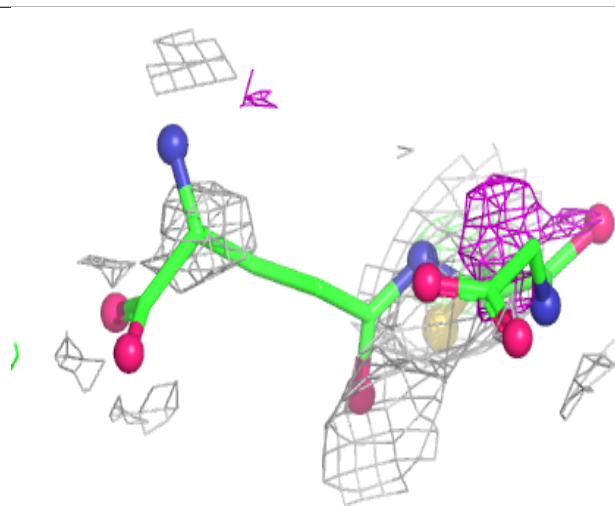
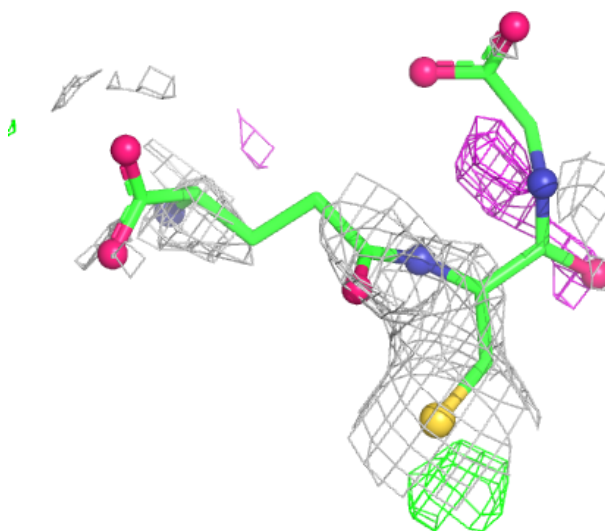
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	GSH	R	404	20/20	0.75	0.17	85,88,96,97	20
3	SO4	O	405	5/5	0.79	0.24	66,67,68,70	5
4	GSH	O	404	20/20	0.82	0.17	69,75,78,78	20
3	SO4	R	405	5/5	0.89	0.12	71,71,71,71	5
3	SO4	R	403	5/5	0.91	0.10	86,87,88,88	0
3	SO4	R	406	5/5	0.91	0.08	76,76,76,76	5
3	SO4	O	402	5/5	0.92	0.12	51,51,51,52	5
2	NAD	R	401	44/44	0.93	0.08	40,50,63,64	0
2	NAD	O	401	44/44	0.93	0.08	44,53,69,70	0
3	SO4	O	403	5/5	0.95	0.07	56,56,57,57	5
3	SO4	R	402	5/5	0.96	0.07	64,64,64,65	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.

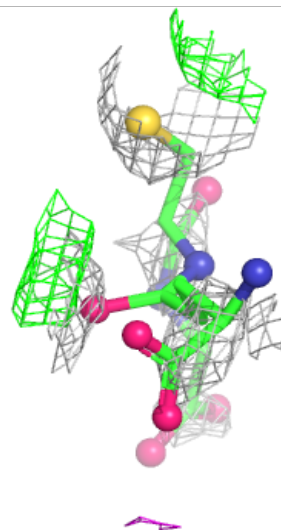
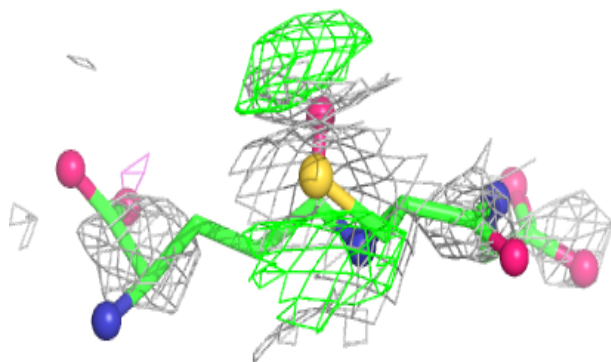
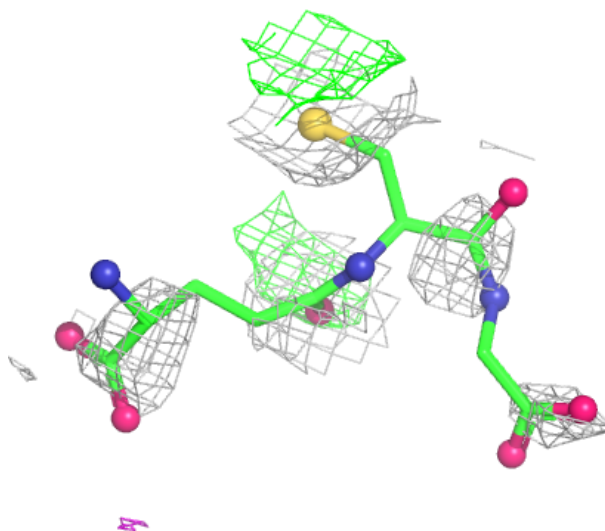
Electron density around GSH R 404:

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



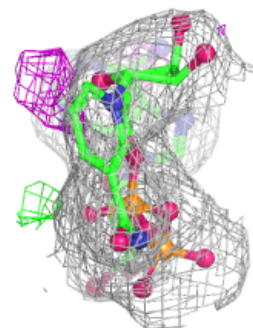
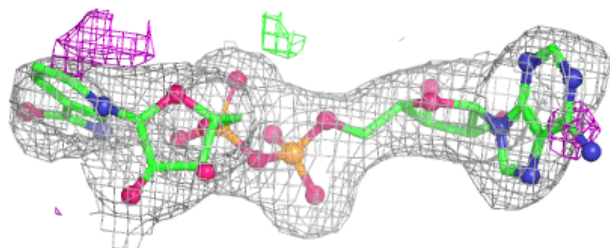
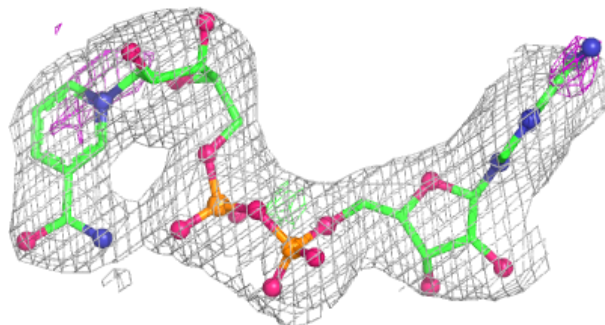
Electron density around GSH O 404:

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

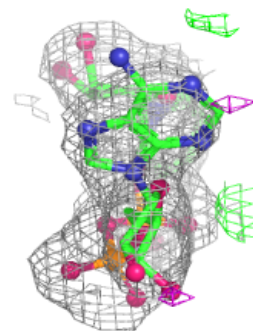
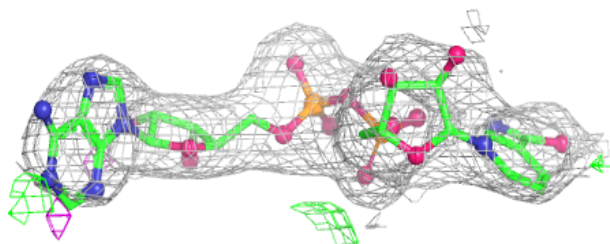
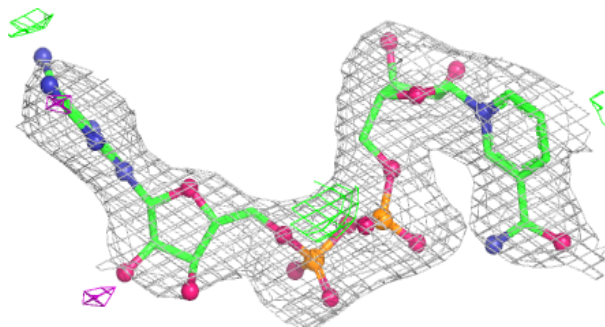


Electron density around NAD R 401:

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

**Electron density around NAD O 401:**

$2mF_o-DF_c$ (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.