



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:57 am BST

PDB ID : 1Q7G
Title : Homoserine Dehydrogenase in complex with suicide inhibitor complex NAD-5-hydroxy-4-Oxonorvaline
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Deposited on : 2003-08-18
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

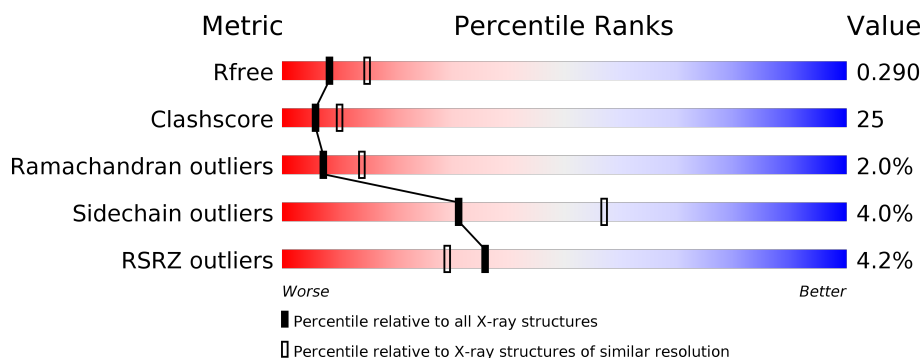
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	359	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>41%</div> <div>.</div> </div> </div>
1	B	359	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>37%</div> <div>.</div> </div> </div>

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	NHO	A	361[B]	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5571 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.

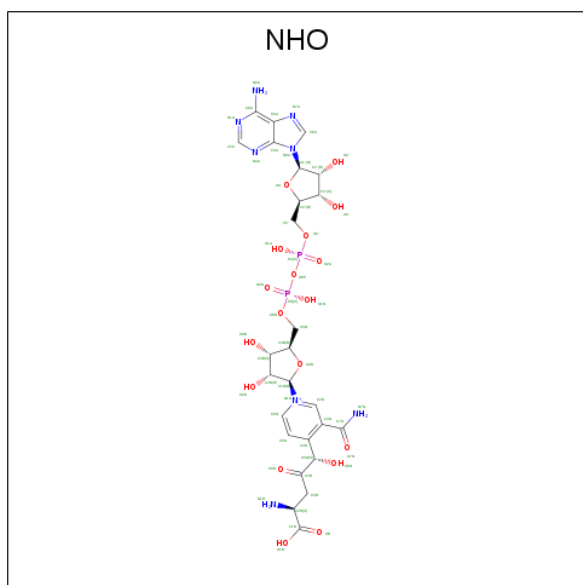
- Molecule 1 is a protein called Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			
1	B	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE-5-HYDROXY-4-OXONOR VALINE (three-letter code: NHO) (formula: $C_{26}H_{35}N_8O_{18}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			108	52	16	36	4		

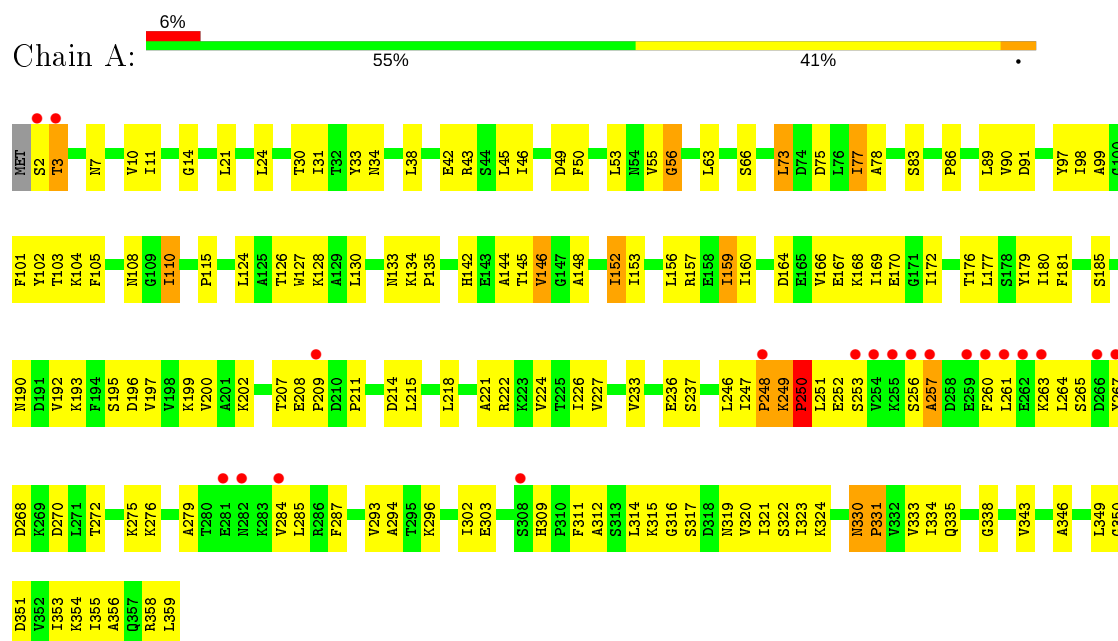
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	20	Total	O	0	0
			20	20		

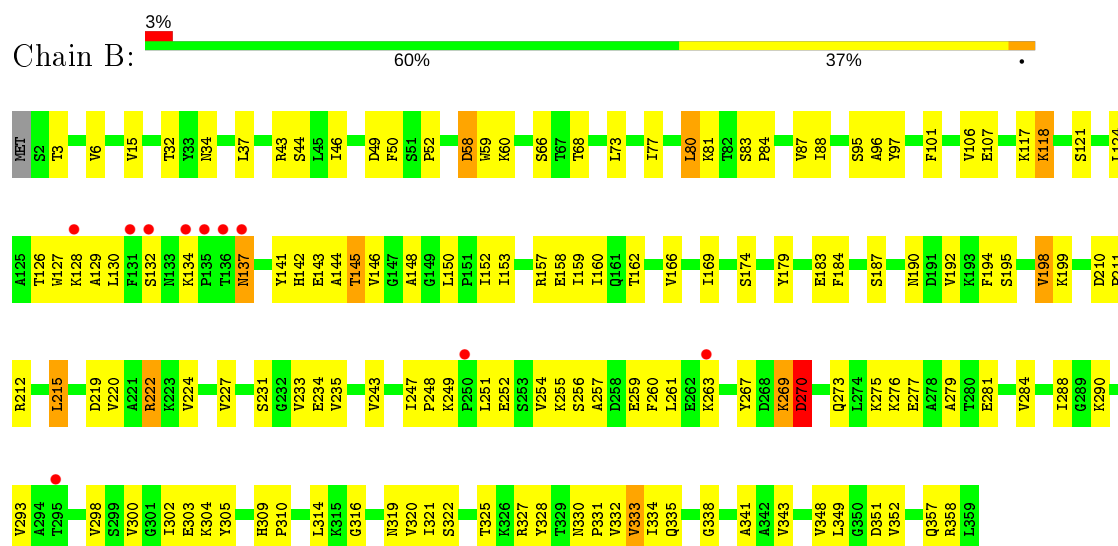
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Homoserine dehydrogenase



- Molecule 1: Homoserine dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.86 Å 80.86 Å 248.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.43 – 2.60 49.33 – 2.61	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.43-2.60) 91.8 (49.33-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.306 0.226 , 0.290	Depositor DCC
R_{free} test set	2548 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5571	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: NA, NHO

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	0.39	0/2757	0.65	0/3741
1	B	0.42	0/2757	0.66	0/3741
All	All	0.40	0/5514	0.65	0/7482

There are no bond length outliers.

There are no bond angle outliers.

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	2710	0	2782	160	0
1	B	2710	0	2782	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	108	0	64	2	0
4	A	21	0	0	1	0
4	B	20	0	0	3	0
All	All	5571	0	5628	279	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 25.

All (279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:HG21	1:A:211:PRO:HG3	1.49	0.95
1:A:159:ILE:HG23	1:A:164:ASP:HB3	1.51	0.93
1:B:251:LEU:HD21	1:B:263:LYS:HD2	1.51	0.91
1:A:207:THR:HG22	1:A:208:GLU:O	1.72	0.88
1:A:314:LEU:HD21	1:A:320:VAL:HG11	1.60	0.83
1:A:89:LEU:HB2	1:A:110:ILE:HD11	1.61	0.82
1:B:142:HIS:HD2	1:B:145:THR:HG21	1.42	0.82
1:B:15:VAL:HG12	1:B:341:ALA:HB2	1.63	0.81
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.45	0.81
1:A:77:ILE:HD13	1:A:104:LYS:HG2	1.63	0.79
1:A:309:HIS:HD2	1:A:311:PHE:H	1.28	0.79
1:B:77:ILE:O	1:B:81:LYS:HG3	1.85	0.76
1:A:142:HIS:HE1	1:A:157:ARG:HH22	1.31	0.76
1:A:207:THR:HG22	1:A:208:GLU:N	2.02	0.74
1:B:96:ALA:HB2	1:B:118:LYS:HD2	1.69	0.74
1:A:77:ILE:CD1	1:A:104:LYS:HG2	2.18	0.73
1:B:106:VAL:HG12	1:B:137:ASN:HB2	1.71	0.72
1:A:167:GLU:HA	1:A:293:VAL:HG21	1.70	0.72
1:A:77:ILE:HD11	1:A:108:ASN:ND2	2.06	0.71
1:A:86:PRO:HB3	1:A:359:LEU:HD13	1.71	0.71
1:A:159:ILE:HD12	1:A:164:ASP:OD2	1.91	0.70
1:A:309:HIS:CD2	1:A:311:PHE:H	2.09	0.69
1:B:166:VAL:HA	1:B:325:THR:HG22	1.73	0.69
1:A:38:LEU:HD23	1:A:45:LEU:HD12	1.75	0.69
1:B:159:ILE:O	1:B:162:THR:HB	1.93	0.69
1:B:107:GLU:HA	1:B:137:ASN:HB3	1.74	0.69
1:B:144:ALA:HA	1:B:148:ALA:O	1.92	0.68
1:A:247:ILE:O	1:A:249:LYS:N	2.26	0.68
1:A:167:GLU:HA	1:A:293:VAL:CG2	2.23	0.67
1:A:249:LYS:HA	1:A:249:LYS:HE2	1.77	0.67
1:A:350:GLY:O	1:A:354:LYS:HG3	1.95	0.67
1:A:142:HIS:HB2	1:A:145:THR:HG23	1.76	0.67
1:A:346:ALA:CB	1:B:162:THR:HG21	2.24	0.67
1:B:145:THR:HG23	1:B:146:VAL:HG23	1.75	0.67
1:A:167:GLU:O	1:A:293:VAL:HG22	1.95	0.66
1:A:346:ALA:HB1	1:B:162:THR:HG21	1.78	0.65
1:B:190:ASN:HD22	1:B:275:LYS:NZ	1.94	0.65
1:A:314:LEU:HD21	1:A:320:VAL:CG1	2.26	0.65
1:A:38:LEU:HB3	1:A:45:LEU:HB2	1.78	0.65
1:B:255:LYS:HG3	1:B:256:SER:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:CG2	1:A:208:GLU:N	2.60	0.65
1:B:195:SER:O	1:B:199:LYS:HB2	1.97	0.65
1:B:142:HIS:O	1:B:145:THR:HB	1.97	0.64
4:A:510:HOH:O	1:B:343:VAL:CG1	2.45	0.64
1:A:343:VAL:HG13	1:B:328:TYR:OH	1.98	0.64
1:B:288:ILE:HD13	1:B:305:TYR:OH	1.98	0.63
1:B:34:ASN:HD21	1:B:52:PRO:CA	2.12	0.63
1:B:212:ARG:HG2	1:B:247:ILE:HD13	1.80	0.63
1:B:222:ARG:NH1	1:B:222:ARG:HG3	2.10	0.63
1:B:130:LEU:HA	4:B:518:HOH:O	1.97	0.63
1:B:194:PHE:O	1:B:198:VAL:HG12	1.99	0.62
1:A:324:LYS:CG	1:A:331:PRO:HG3	2.30	0.61
1:B:255:LYS:HG3	1:B:256:SER:H	1.64	0.61
1:B:142:HIS:HE1	1:B:157:ARG:HH21	1.47	0.61
1:A:252:GLU:HG3	1:A:253:SER:H	1.65	0.61
1:B:166:VAL:HG13	1:B:293:VAL:HG21	1.83	0.61
1:A:196:ASP:O	1:A:200:VAL:HG23	2.00	0.61
1:A:73:LEU:HD23	1:A:97:TYR:CE2	2.36	0.61
1:A:293:VAL:HG23	1:A:294:ALA:N	2.16	0.60
1:B:43:ARG:HD2	1:B:66:SER:O	2.01	0.60
1:A:193:LYS:HB2	1:A:196:ASP:OD2	2.02	0.60
1:B:117:LYS:HE3	1:B:219:ASP:OD2	2.01	0.60
1:B:127:TRP:O	1:B:130:LEU:HB3	2.02	0.60
1:B:142:HIS:CD2	1:B:145:THR:HG21	2.31	0.60
1:B:59:TRP:CH2	1:B:60:LYS:HE3	2.36	0.60
1:A:249:LYS:HE2	1:A:249:LYS:CA	2.32	0.59
1:A:207:THR:HG21	1:A:211:PRO:CG	2.28	0.58
1:A:86:PRO:CB	1:A:359:LEU:HD13	2.33	0.58
1:A:156:LEU:HD21	1:A:323:ILE:HD13	1.85	0.58
1:A:249:LYS:O	1:A:250:PRO:O	2.20	0.58
1:A:77:ILE:HD11	1:A:108:ASN:CG	2.24	0.58
1:B:174:SER:HB2	1:B:220:VAL:HG12	1.86	0.57
1:A:89:LEU:CB	1:A:110:ILE:HD11	2.33	0.57
1:A:202:LYS:HA	1:A:207:THR:HB	1.85	0.57
1:A:272:THR:O	1:A:276:LYS:HG2	2.03	0.57
1:B:34:ASN:ND2	1:B:52:PRO:HG3	2.19	0.57
1:B:169:ILE:HG21	1:B:227:VAL:HG11	1.87	0.57
1:A:142:HIS:CE1	1:A:157:ARG:HH22	2.20	0.57
1:A:207:THR:CG2	1:A:208:GLU:H	2.18	0.57
1:A:172:ILE:HB	1:A:320:VAL:HG22	1.86	0.57
1:B:314:LEU:HD11	1:B:320:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:VAL:O	1:B:352:VAL:HG23	2.03	0.56
1:A:251:LEU:HD11	1:A:263:LYS:HZ3	1.70	0.56
1:A:55:VAL:O	1:A:56:GLY:C	2.43	0.56
1:B:166:VAL:HG11	1:B:231:SER:HB3	1.87	0.56
1:A:160:ILE:HD11	1:A:166:VAL:HG23	1.87	0.56
1:A:185:SER:HB3	1:A:275:LYS:HG3	1.87	0.56
1:A:21:LEU:HD11	1:A:38:LEU:HD11	1.88	0.56
1:B:73:LEU:O	1:B:77:ILE:HD12	2.06	0.56
1:A:221:ALA:O	1:A:224:VAL:HG12	2.06	0.56
1:B:34:ASN:HD21	1:B:52:PRO:HA	1.71	0.56
1:A:169:ILE:HG21	1:A:227:VAL:HG11	1.88	0.56
1:A:89:LEU:HD22	1:A:105:PHE:CE2	2.41	0.55
1:A:126:THR:O	1:A:130:LEU:HG	2.06	0.55
1:A:324:LYS:HG3	1:A:331:PRO:HG3	1.88	0.55
1:A:193:LYS:HE2	1:A:268:ASP:OD2	2.07	0.55
1:A:7:ASN:HD22	1:A:34:ASN:HB2	1.71	0.55
1:B:233:VAL:O	1:B:235:VAL:HG23	2.07	0.55
1:B:153:ILE:O	1:B:157:ARG:HG2	2.07	0.54
1:B:212:ARG:HD2	1:B:260:PHE:CD1	2.42	0.54
1:B:141:TYR:HB3	1:B:351:ASP:OD2	2.07	0.54
1:A:127:TRP:HA	1:A:130:LEU:HD12	1.88	0.54
1:A:7:ASN:ND2	1:A:34:ASN:HB2	2.22	0.54
1:A:2:SER:HB2	1:B:358:ARG:HG2	1.88	0.54
1:B:184:PHE:O	1:B:275:LYS:HE3	2.07	0.54
1:A:142:HIS:HB2	1:A:145:THR:CG2	2.37	0.54
1:A:334:ILE:HG23	1:B:334:ILE:CD1	2.38	0.54
1:B:233:VAL:O	1:B:235:VAL:N	2.41	0.54
1:A:105:PHE:O	1:A:110:ILE:HG23	2.08	0.54
1:A:322:SER:OG	1:A:331:PRO:HB3	2.08	0.54
1:B:80:LEU:HG	1:B:87:VAL:HG11	1.90	0.54
1:A:309:HIS:CD2	1:A:311:PHE:HB2	2.43	0.53
1:B:145:THR:CG2	1:B:146:VAL:HG23	2.37	0.53
1:B:162:THR:HG22	1:B:327:ARG:NH2	2.22	0.53
1:B:121:SER:OG	1:B:222:ARG:HD3	2.08	0.53
1:A:248:PRO:HD2	1:A:260:PHE:HE1	1.73	0.53
1:B:159:ILE:HG13	1:B:160:ILE:N	2.23	0.53
1:A:152:ILE:CG1	1:A:153:ILE:N	2.71	0.53
1:B:73:LEU:HD13	1:B:101:PHE:CD1	2.43	0.53
1:A:333:VAL:HB	1:B:335:GLN:HG2	1.91	0.53
1:B:37:LEU:HD11	1:B:46:ILE:HG12	1.89	0.53
1:B:6:VAL:HG11	1:B:88:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLU:HG2	1:B:281:GLU:OE2	2.08	0.53
1:B:166:VAL:HG12	4:B:514:HOH:O	2.08	0.52
1:A:14:GLY:HA3	3:A:361[A]:NHO:H5'2	1.91	0.52
1:A:251:LEU:HD23	1:A:251:LEU:O	2.10	0.52
1:A:349:LEU:O	1:A:353:ILE:HG13	2.09	0.52
1:B:49:ASP:O	1:B:50:PHE:HB2	2.10	0.52
1:A:45:LEU:HD13	1:A:55:VAL:HG11	1.92	0.52
1:A:14:GLY:HA3	3:A:361[B]:NHO:H5'2	1.92	0.51
1:B:184:PHE:CZ	1:B:275:LYS:HD2	2.45	0.51
1:A:190:ASN:HD22	1:A:192:VAL:CG2	2.24	0.51
1:A:105:PHE:HD2	1:A:110:ILE:HD13	1.74	0.51
1:B:243:VAL:HG22	1:B:300:VAL:HG13	1.93	0.51
1:B:284:VAL:O	1:B:304:LYS:HA	2.11	0.51
1:A:144:ALA:HA	1:A:148:ALA:O	2.10	0.51
1:A:91:ASP:O	1:A:115:PRO:HD2	2.11	0.51
1:B:124:LEU:O	1:B:128:LYS:HG2	2.11	0.51
1:B:302:ILE:HG22	1:B:303:GLU:N	2.25	0.51
1:A:190:ASN:HD22	1:A:192:VAL:HG23	1.75	0.51
1:A:211:PRO:O	1:A:215:LEU:HG	2.11	0.50
1:B:137:ASN:H	1:B:137:ASN:ND2	2.10	0.50
1:B:143:GLU:C	1:B:145:THR:H	2.15	0.50
1:A:251:LEU:HD11	1:A:263:LYS:NZ	2.26	0.50
1:A:159:ILE:HG23	1:A:164:ASP:CB	2.35	0.50
1:A:233:VAL:HA	1:A:296:LYS:HE3	1.94	0.49
1:A:222:ARG:O	1:A:226:ILE:HG13	2.12	0.49
1:B:220:VAL:O	1:B:224:VAL:HG23	2.12	0.49
1:B:248:PRO:HB3	1:B:267:TYR:CD2	2.48	0.49
1:B:3:THR:HG21	1:B:32:THR:OG1	2.13	0.49
1:A:358:ARG:HG3	1:B:357:GLN:HB3	1.95	0.49
1:B:190:ASN:HD21	1:B:192:VAL:HB	1.78	0.49
1:B:134:LYS:HB2	1:B:137:ASN:ND2	2.27	0.49
1:B:254:VAL:HG13	1:B:259:GLU:OE2	2.13	0.49
1:B:37:LEU:CD1	1:B:46:ILE:HG12	2.43	0.49
1:A:169:ILE:O	1:A:170:GLU:HB3	2.13	0.48
1:B:150:LEU:HB2	1:B:152:ILE:HD12	1.94	0.48
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.77	0.48
1:A:302:ILE:HG22	1:A:303:GLU:N	2.27	0.48
1:A:176:THR:O	1:A:180:ILE:HG13	2.13	0.48
1:A:50:PHE:CE2	1:A:83:SER:HB2	2.48	0.48
1:B:215:LEU:HD23	1:B:215:LEU:N	2.29	0.48
1:B:254:VAL:CG1	1:B:259:GLU:HB3	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HG22	1:A:30:THR:O	2.13	0.48
1:A:335:GLN:O	1:B:332:VAL:O	2.30	0.48
1:A:320:VAL:HG12	1:A:335:GLN:CB	2.43	0.48
1:A:261:LEU:O	1:A:264:LEU:HB3	2.13	0.48
1:A:146:VAL:O	1:A:146:VAL:HG22	2.14	0.47
1:B:212:ARG:HG3	1:B:260:PHE:CZ	2.49	0.47
1:B:332:VAL:HG12	1:B:332:VAL:O	2.14	0.47
1:B:95:SER:OG	1:B:97:TYR:HB3	2.14	0.47
1:A:105:PHE:CD2	1:A:110:ILE:HD13	2.50	0.47
1:B:269:LYS:O	1:B:273:GLN:HG3	2.14	0.47
1:B:137:ASN:HD22	1:B:137:ASN:H	1.62	0.47
1:B:267:TYR:CD1	1:B:267:TYR:N	2.83	0.47
1:A:152:ILE:HD12	1:A:321:ILE:CD1	2.45	0.47
1:A:3:THR:O	1:A:31:ILE:HG12	2.14	0.47
1:B:121:SER:OG	1:B:222:ARG:CD	2.63	0.47
1:B:58:ASP:OD2	1:B:60:LYS:HB2	2.13	0.47
1:A:302:ILE:CG2	1:A:303:GLU:N	2.78	0.47
1:A:134:LYS:CG	1:A:135:PRO:HD2	2.45	0.46
1:A:177:LEU:HD13	1:A:287:PHE:CD2	2.50	0.46
1:A:11:ILE:HG21	1:A:98:ILE:HD13	1.97	0.46
1:A:309:HIS:HD2	1:A:311:PHE:HB2	1.79	0.46
1:A:330:ASN:HA	1:A:330:ASN:HD22	1.58	0.46
1:A:156:LEU:O	1:A:160:ILE:HG12	2.14	0.46
1:A:293:VAL:HG23	1:A:294:ALA:H	1.79	0.46
1:B:276:LYS:O	1:B:279:ALA:N	2.47	0.46
1:A:249:LYS:HB3	1:A:250:PRO:CD	2.46	0.46
1:B:184:PHE:CE1	1:B:275:LYS:HD2	2.50	0.46
1:A:195:SER:O	1:A:199:LYS:HE3	2.16	0.46
1:B:179:TYR:CZ	1:B:183:GLU:HG3	2.50	0.46
1:B:190:ASN:ND2	1:B:275:LYS:NZ	2.61	0.46
1:A:180:ILE:HG23	1:A:197:VAL:CG1	2.46	0.45
1:A:334:ILE:HG23	1:B:334:ILE:HD13	1.97	0.45
1:A:324:LYS:HG2	1:A:331:PRO:HG3	1.97	0.45
1:B:309:HIS:ND1	1:B:310:PRO:HD2	2.30	0.45
1:A:152:ILE:HG13	1:A:153:ILE:N	2.31	0.45
1:A:221:ALA:HA	1:A:224:VAL:HG12	1.99	0.45
1:A:73:LEU:O	1:A:77:ILE:CG2	2.64	0.45
1:A:99:ALA:HA	1:A:102:TYR:CE2	2.52	0.45
1:A:285:LEU:HD22	1:A:302:ILE:HG21	1.98	0.45
1:B:290:LYS:O	1:B:298:VAL:HA	2.17	0.45
1:A:75:ASP:O	1:A:78:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:O	1:B:68:THR:HB	2.16	0.44
1:A:207:THR:HG23	1:A:211:PRO:HA	1.98	0.44
1:B:96:ALA:HB2	1:B:118:LYS:CD	2.44	0.44
1:A:172:ILE:HB	1:A:320:VAL:CG2	2.48	0.44
1:B:106:VAL:CG1	1:B:137:ASN:HB2	2.42	0.44
1:B:96:ALA:CB	1:B:118:LYS:HD2	2.44	0.44
1:B:349:LEU:O	1:B:352:VAL:HB	2.18	0.44
1:B:270:ASP:N	1:B:270:ASP:OD2	2.45	0.44
1:A:208:GLU:HG2	1:A:214:ASP:OD2	2.18	0.44
1:B:330:ASN:HB2	4:B:507:HOH:O	2.18	0.43
1:B:83:SER:HA	1:B:84:PRO:HD3	1.83	0.43
1:A:49:ASP:O	1:A:50:PHE:HB2	2.17	0.43
1:B:142:HIS:HE1	1:B:157:ARG:NH2	2.12	0.43
1:B:320:VAL:HG13	1:B:335:GLN:HB3	2.01	0.43
1:A:250:PRO:O	1:A:251:LEU:C	2.57	0.43
1:A:276:LYS:O	1:A:279:ALA:HB3	2.18	0.43
1:A:319:ASN:CG	1:A:338:GLY:HA3	2.38	0.43
1:B:73:LEU:HD13	1:B:101:PHE:CG	2.54	0.43
1:B:321:ILE:O	1:B:333:VAL:HA	2.19	0.43
1:A:267:TYR:N	1:A:267:TYR:CD2	2.86	0.43
1:A:63:LEU:O	1:A:66:SER:HB3	2.18	0.43
1:B:249:LYS:O	1:B:252:GLU:HB2	2.18	0.43
1:A:320:VAL:HG12	1:A:335:GLN:HB2	2.00	0.43
1:B:126:THR:O	1:B:129:ALA:HB3	2.18	0.43
1:A:315:LYS:O	1:A:316:GLY:C	2.56	0.43
1:B:143:GLU:C	1:B:145:THR:N	2.71	0.43
1:A:10:VAL:HG22	1:A:90:VAL:HB	2.01	0.43
1:A:208:GLU:O	1:A:209:PRO:C	2.57	0.43
1:A:354:LYS:HE3	1:B:158:GLU:OE2	2.18	0.43
1:B:332:VAL:O	1:B:333:VAL:O	2.37	0.43
1:B:148:ALA:HB2	1:B:338:GLY:C	2.39	0.42
1:B:276:LYS:O	1:B:279:ALA:HB3	2.19	0.42
1:A:169:ILE:CG2	1:A:170:GLU:N	2.83	0.42
1:A:284:VAL:HG22	1:A:285:LEU:H	1.84	0.42
1:A:134:LYS:HG3	1:A:135:PRO:HD2	2.01	0.42
1:A:236:GLU:O	1:A:237:SER:HB3	2.18	0.42
1:A:351:ASP:O	1:A:355:ILE:HG13	2.20	0.42
1:B:162:THR:HG22	1:B:327:ARG:HH22	1.83	0.42
1:B:257:ALA:O	1:B:261:LEU:HG	2.20	0.42
1:A:168:LYS:HE3	1:A:324:LYS:HD2	2.01	0.42
1:B:134:LYS:HB2	1:B:137:ASN:CG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:VAL:HG11	1:B:231:SER:CB	2.49	0.42
1:B:322:SER:OG	1:B:331:PRO:HB3	2.20	0.42
1:B:243:VAL:HG13	1:B:300:VAL:HG22	2.01	0.42
1:A:45:LEU:CD1	1:A:55:VAL:HG11	2.49	0.42
1:A:124:LEU:O	1:A:128:LYS:HG3	2.20	0.42
1:B:314:LEU:HD11	1:B:320:VAL:CG2	2.48	0.42
1:A:157:ARG:NH1	1:A:157:ARG:HG3	2.34	0.41
1:A:11:ILE:HG21	1:A:98:ILE:CD1	2.51	0.41
1:A:152:ILE:HD12	1:A:321:ILE:HD13	2.02	0.41
1:B:137:ASN:ND2	1:B:137:ASN:N	2.67	0.41
1:B:276:LYS:O	1:B:277:GLU:C	2.59	0.41
1:A:202:LYS:HD2	1:A:261:LEU:HD11	2.02	0.41
1:B:332:VAL:O	1:B:333:VAL:C	2.58	0.41
1:A:207:THR:CG2	1:A:211:PRO:HA	2.50	0.41
1:A:167:GLU:HA	1:A:293:VAL:HG22	2.01	0.41
1:A:256:SER:O	1:A:257:ALA:C	2.59	0.41
1:B:212:ARG:O	1:B:247:ILE:HD11	2.19	0.41
1:A:319:ASN:O	1:A:335:GLN:HA	2.21	0.41
1:A:33:TYR:HE1	1:A:356:ALA:HB2	1.86	0.41
1:A:42:GLU:HG3	1:A:43:ARG:NE	2.36	0.41
1:A:251:LEU:HD13	1:A:267:TYR:OH	2.20	0.41
1:A:293:VAL:CG2	1:A:294:ALA:N	2.83	0.41
1:A:101:PHE:O	1:A:102:TYR:C	2.60	0.41
1:A:124:LEU:HG	1:A:128:LYS:HE3	2.02	0.41
1:A:169:ILE:HG22	1:A:170:GLU:N	2.36	0.41
1:A:73:LEU:O	1:A:77:ILE:HG22	2.20	0.41
1:A:179:TYR:HB2	1:A:317:SER:HB3	2.03	0.40
1:A:181:PHE:HE1	1:A:246:LEU:HD21	1.85	0.40
1:A:53:LEU:HA	1:A:53:LEU:HD23	1.97	0.40
1:A:89:LEU:HD22	1:A:105:PHE:CD2	2.56	0.40
1:B:210:ASP:HA	1:B:211:PRO:HD2	1.94	0.40
1:A:309:HIS:O	1:A:312:ALA:HB3	2.21	0.40
1:B:132:SER:C	1:B:134:LYS:N	2.74	0.40
1:B:137:ASN:HD22	1:B:137:ASN:N	2.18	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	356/359 (99%)	313 (88%)	36 (10%)	7 (2%)	7	14
1	B	356/359 (99%)	315 (88%)	34 (10%)	7 (2%)	7	14
All	All	712/718 (99%)	628 (88%)	70 (10%)	14 (2%)	7	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	PRO
1	A	250	PRO
1	A	257	ALA
1	B	234	GLU
1	B	333	VAL
1	A	56	GLY
1	A	249	LYS
1	A	265	SER
1	B	58	ASP
1	B	269	LYS
1	B	270	ASP
1	B	118	LYS
1	B	316	GLY
1	A	331	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	A	300/301 (100%)	285 (95%)	15 (5%)	24	47
1	B	300/301 (100%)	291 (97%)	9 (3%)	41	67
All	All	600/602 (100%)	576 (96%)	24 (4%)	31	57

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	24	LEU
1	A	46	ILE
1	A	73	LEU
1	A	77	ILE
1	A	103	THR
1	A	110	ILE
1	A	133	ASN
1	A	146	VAL
1	A	152	ILE
1	A	159	ILE
1	A	218	LEU
1	A	250	PRO
1	A	270	ASP
1	A	330	ASN
1	B	80	LEU
1	B	137	ASN
1	B	145	THR
1	B	187	SER
1	B	198	VAL
1	B	215	LEU
1	B	222	ARG
1	B	270	ASP
1	B	319	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	79	HIS
1	A	133	ASN
1	A	137	ASN
1	A	142	HIS
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	190	ASN
1	A	309	HIS
1	A	330	ASN
1	B	7	ASN
1	B	34	ASN
1	B	137	ASN
1	B	142	HIS
1	B	161	GLN
1	B	190	ASN
1	B	330	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NHO	A	361[A]	-	48,58,58	3.09	7 (14%)	54,88,88	1.73	10 (18%)
3	NHO	A	361[B]	-	48,58,58	3.09	7 (14%)	54,88,88	1.73	10 (18%)

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	NHO	A	361[A]	-	-	13/38/78/78	0/5/5/5
3	NHO	A	361[B]	-	1/1/15/15	13/38/78/78	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361[A]	NHO	C3N-C4N	15.21	1.57	1.40
3	A	361[B]	NHO	C3N-C4N	15.08	1.57	1.40
3	A	361[B]	NHO	C5N-C4N	10.50	1.53	1.39
3	A	361[A]	NHO	C5N-C4N	10.39	1.53	1.39
3	A	361[A]	NHO	C4N-C5R	5.74	1.58	1.52
3	A	361[B]	NHO	C2N-N1N	5.70	1.41	1.35
3	A	361[B]	NHO	C4N-C5R	5.68	1.58	1.52
3	A	361[A]	NHO	C2N-N1N	5.61	1.41	1.35
3	A	361[A]	NHO	C4A-N3A	3.31	1.40	1.35
3	A	361[B]	NHO	C4A-N3A	3.29	1.40	1.35
3	A	361[A]	NHO	C6N-N1N	2.99	1.42	1.35
3	A	361[B]	NHO	C6N-N1N	2.95	1.42	1.35
3	A	361[B]	NHO	C2A-N1A	2.44	1.38	1.33
3	A	361[A]	NHO	C2A-N1A	2.43	1.38	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361[A]	NHO	C5N-C4N-C3N	-5.22	112.77	118.83
3	A	361[B]	NHO	C5N-C4N-C3N	-5.21	112.78	118.83
3	A	361[B]	NHO	C5N-C4N-C5R	-5.07	108.44	120.34
3	A	361[A]	NHO	C5N-C4N-C5R	-5.00	108.59	120.34
3	A	361[B]	NHO	C4N-C5R-C4R	4.19	122.42	110.88
3	A	361[A]	NHO	C4N-C5R-C4R	4.18	122.40	110.88
3	A	361[B]	NHO	PN-OPP-PA	-4.16	118.56	132.83
3	A	361[A]	NHO	PN-OPP-PA	-4.14	118.62	132.83
3	A	361[B]	NHO	O4B-C1B-C2B	-3.42	101.92	106.93
3	A	361[A]	NHO	O4B-C1B-C2B	-3.42	101.93	106.93
3	A	361[B]	NHO	O7N-C7N-C3N	-3.03	116.67	120.24
3	A	361[A]	NHO	O7N-C7N-C3N	-3.01	116.70	120.24
3	A	361[B]	NHO	O4'-C1'-C2'	-2.84	102.78	106.93
3	A	361[A]	NHO	O4'-C1'-C2'	-2.83	102.79	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361[B]	NHO	C1'-N9A-C4A	-2.61	122.06	126.64
3	A	361[A]	NHO	C1'-N9A-C4A	-2.57	122.12	126.64
3	A	361[A]	NHO	N6A-C6A-N1A	2.42	123.59	118.57
3	A	361[B]	NHO	N6A-C6A-N1A	2.40	123.55	118.57
3	A	361[B]	NHO	C6N-N1N-C2N	2.36	124.13	121.97
3	A	361[A]	NHO	C6N-N1N-C2N	2.29	124.07	121.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	361[B]	NHO	C5R

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	361[B]	NHO	C5N-C4N-C5R-O5R
3	A	361[B]	NHO	O4R-C4R-C5R-O5R
3	A	361[B]	NHO	N1R-C2R-C3R-C4R
3	A	361[B]	NHO	C1R-C2R-C3R-C4R
3	A	361[A]	NHO	O4R-C4R-C5R-O5R
3	A	361[A]	NHO	C3R-C4R-C5R-O5R
3	A	361[A]	NHO	N1R-C2R-C3R-C4R
3	A	361[A]	NHO	C1R-C2R-C3R-C4R
3	A	361[B]	NHO	C4N-C3N-C7N-O7N
3	A	361[A]	NHO	C4N-C3N-C7N-O7N
3	A	361[B]	NHO	C5'-O5'-PA-OPP
3	A	361[A]	NHO	C5'-O5'-PA-OPP
3	A	361[B]	NHO	PN-OPP-PA-O2A
3	A	361[B]	NHO	O4R-C4R-C5R-C4N
3	A	361[A]	NHO	PN-OPP-PA-O2A
3	A	361[A]	NHO	O4R-C4R-C5R-C4N
3	A	361[B]	NHO	C5N-C4N-C5R-C4R
3	A	361[A]	NHO	C5N-C4N-C5R-C4R
3	A	361[B]	NHO	C2R-C3R-C4R-C5R
3	A	361[A]	NHO	C2R-C3R-C4R-C5R
3	A	361[B]	NHO	C3R-C4R-C5R-C4N
3	A	361[A]	NHO	C3R-C4R-C5R-C4N
3	A	361[B]	NHO	C4N-C3N-C7N-N7N
3	A	361[A]	NHO	C4N-C3N-C7N-N7N
3	A	361[B]	NHO	C5'-O5'-PA-O2A
3	A	361[A]	NHO	C5'-O5'-PA-O2A

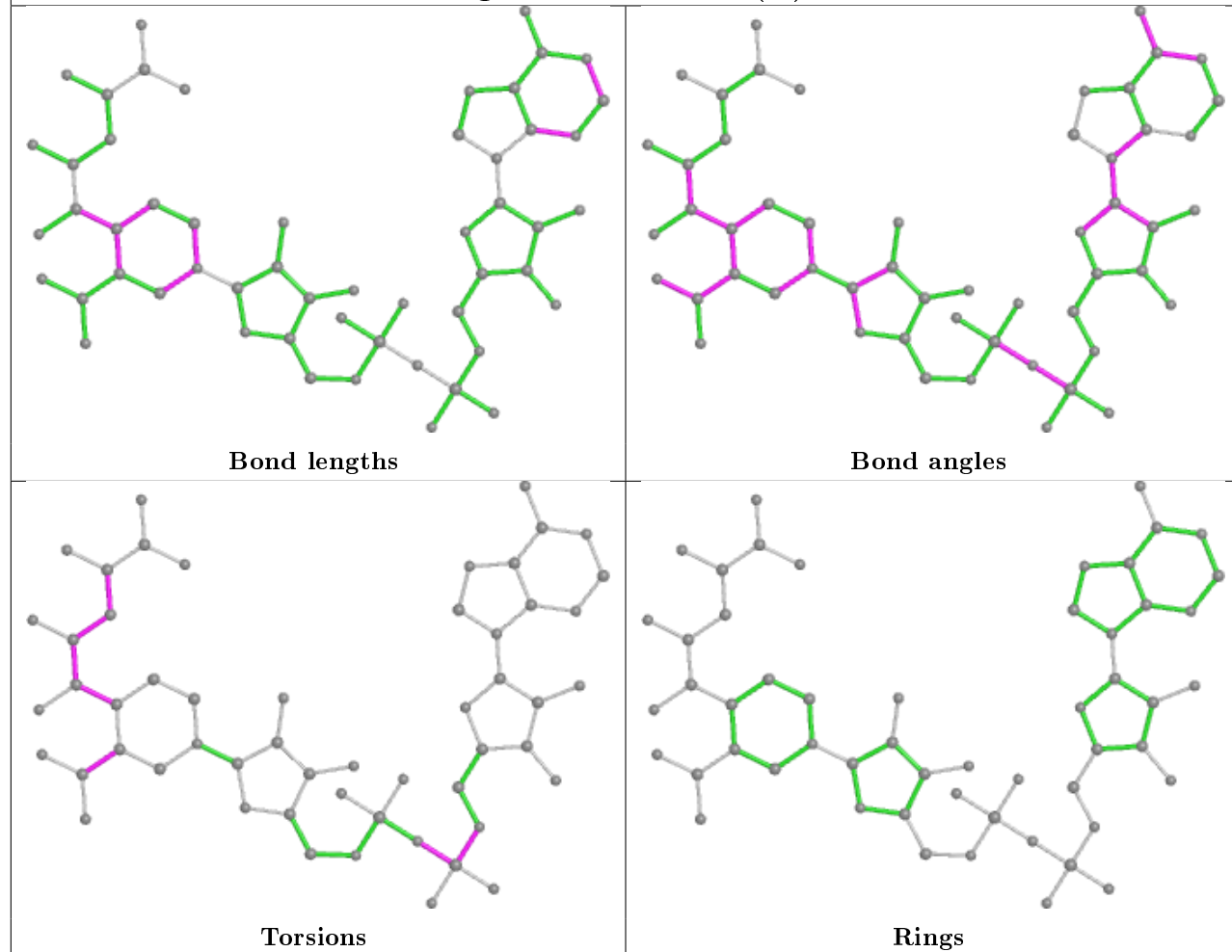
There are no ring outliers.

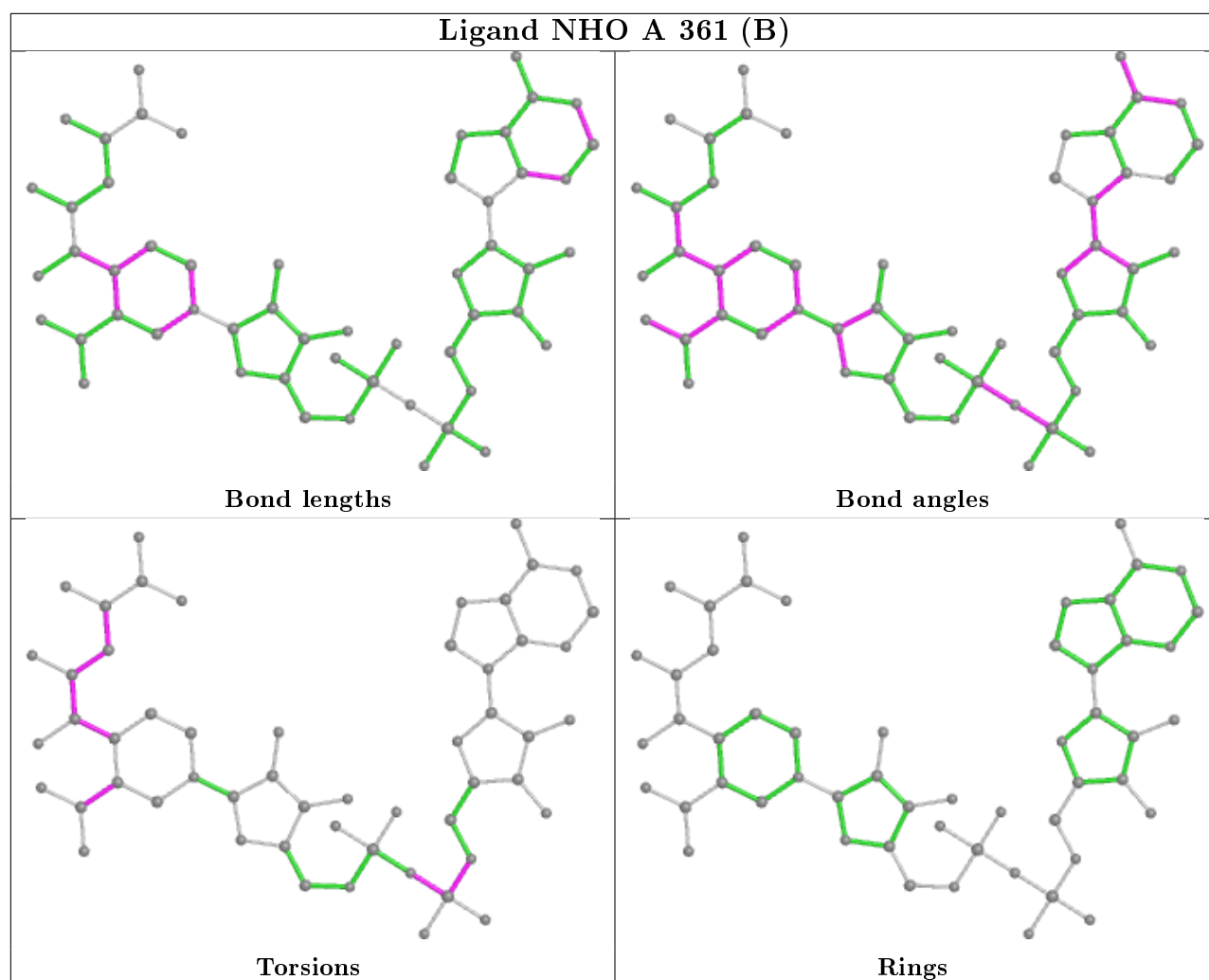
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	361[A]	NHO	1	0
3	A	361[B]	NHO	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.

Ligand NHO A 361 (A)





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	358/359 (99%)	0.13	20 (5%) 24 19	11, 29, 76, 89	0
1	B	358/359 (99%)	-0.02	10 (2%) 53 46	13, 29, 46, 70	0
All	All	716/718 (99%)	0.05	30 (4%) 36 29	11, 29, 69, 89	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	THR	7.8
1	A	254	VAL	6.3
1	B	132	SER	5.8
1	B	136	THR	5.0
1	A	262	GLU	4.7
1	A	263	LYS	4.0
1	A	2	SER	3.9
1	B	263	LYS	3.9
1	A	261	LEU	3.2
1	A	267	TYR	3.0
1	A	248	PRO	2.9
1	A	266	ASP	2.8
1	B	295	THR	2.7
1	A	256	SER	2.7
1	A	282	ASN	2.6
1	B	131	PHE	2.6
1	A	255	LYS	2.4
1	B	134	LYS	2.4
1	B	250	PRO	2.4
1	A	308	SER	2.3
1	A	257	ALA	2.3
1	B	137	ASN	2.3
1	A	259	GLU	2.3
1	A	260	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	284	VAL	2.1
1	A	281	GLU	2.1
1	B	128	LYS	2.1
1	B	135	PRO	2.1
1	A	253	SER	2.1
1	A	209	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

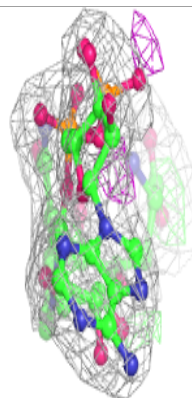
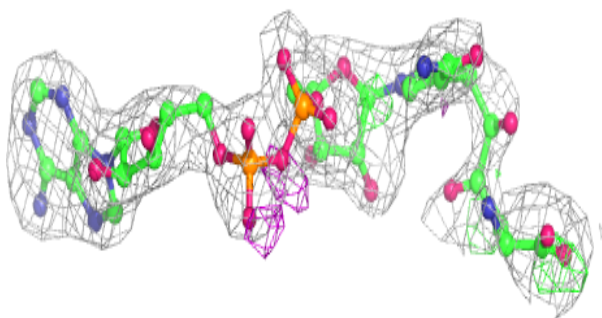
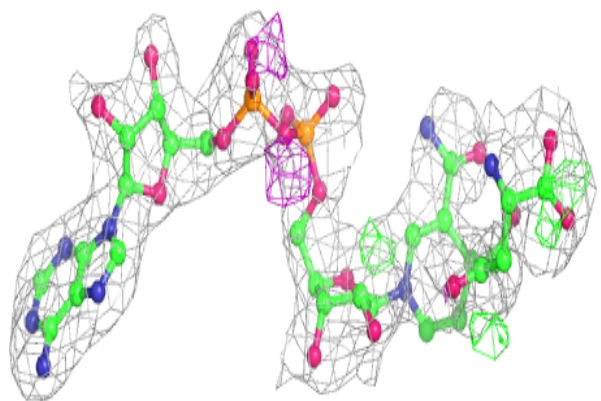
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	B	501	1/1	0.86	0.26	34,34,34,34	0
3	NHO	A	361[B]	54/54	0.91	0.20	22,40,55,55	54
3	NHO	A	361[A]	54/54	0.91	0.20	22,40,55,55	54
2	NA	A	500	1/1	0.98	0.19	25,25,25,25	0

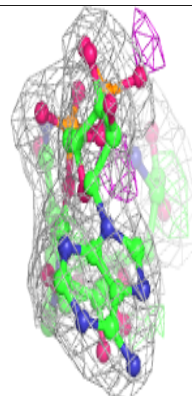
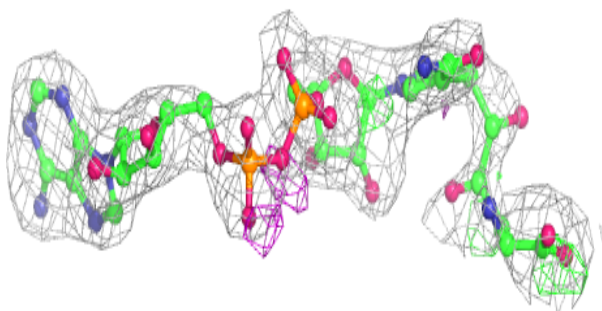
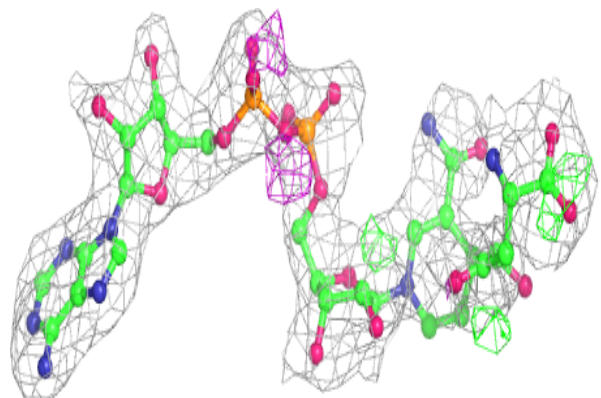
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NHO A 361 (B):

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

**Electron density around NHO A 361 (A):**

$2mF_o-DF_c$ (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.