



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:39 PM UTC

PDB ID : 1Q7G / pdb_00001q7g
Title : Homoserine Dehydrogenase in complex with suicide inhibitor complex NAD-5-hydroxy-4-Oxonorvaline
Authors : Jacques, S.L.; Mirza, I.A.; Ejim, L.; Koteva, K.; Hughes, D.W.; Green, K.; Kinach, R.; Honek, J.F.; Lai, H.K.; Berghuis, A.M.; Wright, G.D.
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 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

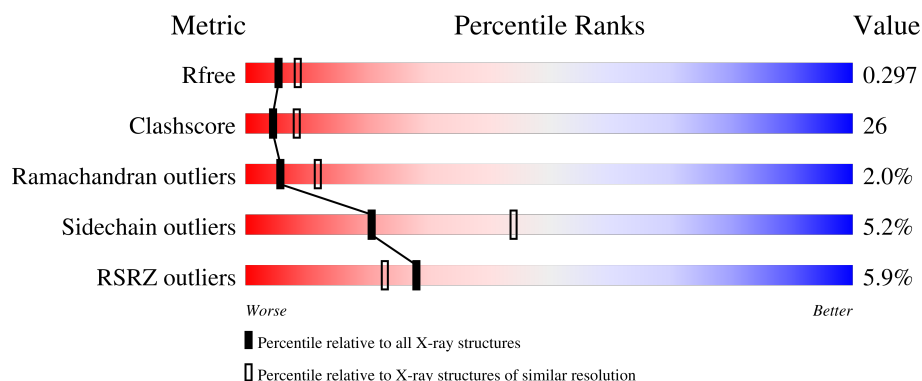
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	8% 52% 43% ..
1	B	359	3% 57% 36% 7% .

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.

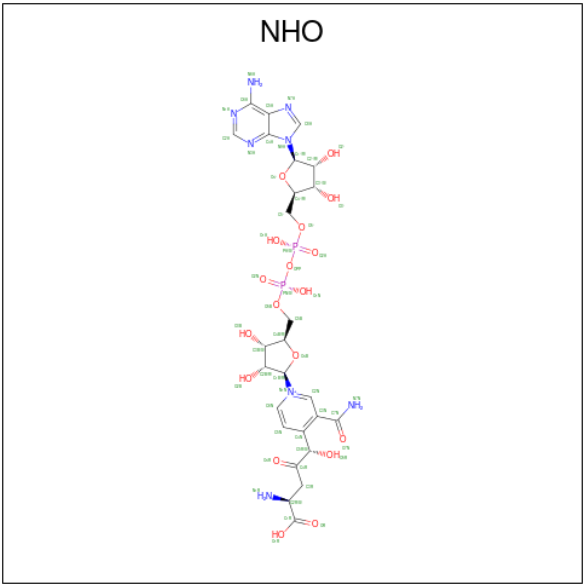
- Molecule 1 is a protein called Homoserine dehydrogenase.

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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE-5-HYDROXY-4-OXONOR VALINE (CCD ID: NHO) (formula: C₂₆H₃₅N₈O₁₈P₂).



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

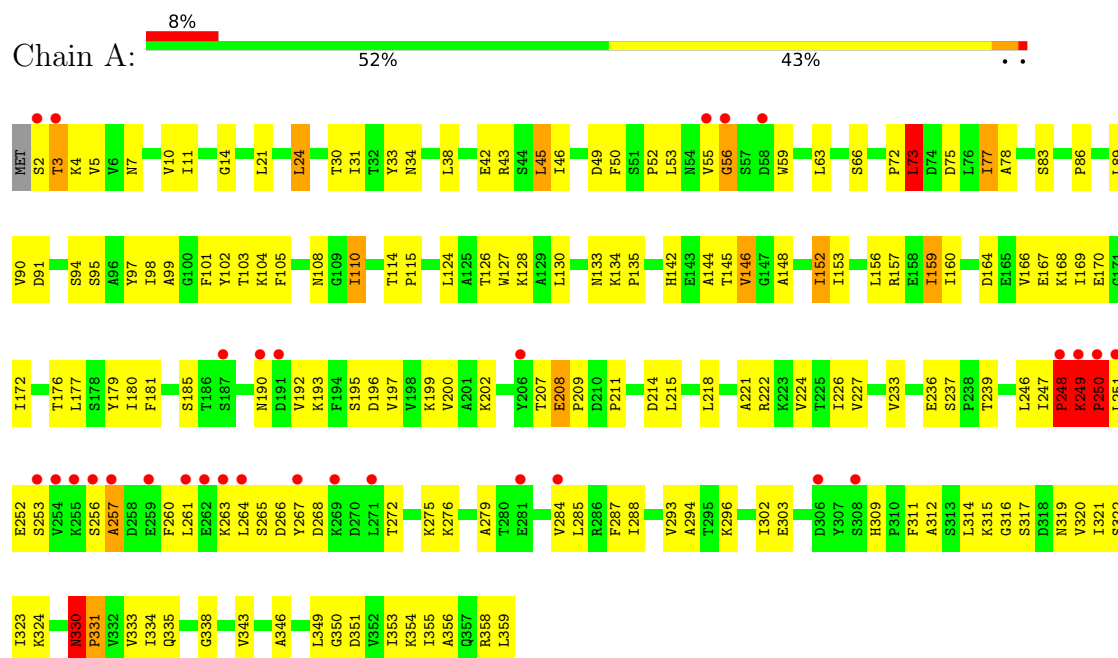
- Molecule 4 is water.

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

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: Homoserine dehydrogenase



V352	
	Q357
	R358
	L359

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.86Å 80.86Å 248.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.43 – 2.60 40.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.43-2.60) 91.8 (40.43-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.306 0.234 , 0.297	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)	0.38 , 55.1	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	0.48	0/2757	1.03	14/3741 (0.4%)
1	B	0.49	0/2757	1.03	15/3741 (0.4%)
All	All	0.48	0/5514	1.03	29/7482 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	THR	N-CA-C	9.76	117.01	108.22
1	A	4	LYS	N-CA-C	7.96	119.65	110.97
1	A	208	GLU	N-CA-C	-7.79	100.19	110.40
1	A	330	ASN	CA-C-N	7.72	129.50	119.84
1	A	330	ASN	C-N-CA	7.72	129.50	119.84
1	A	5	VAL	N-CA-C	7.68	118.86	108.11
1	B	257	ALA	N-CA-C	-7.47	104.15	113.18
1	B	319	ASN	N-CA-C	-7.12	99.67	110.14
1	B	114	THR	N-CA-C	6.86	114.31	108.13
1	A	94	SER	N-CA-C	-6.81	104.28	112.59
1	B	115	PRO	N-CA-C	-6.68	105.23	114.98
1	A	288	ILE	N-CA-C	6.54	116.80	108.82
1	A	45	LEU	N-CA-C	-6.48	98.67	109.24
1	B	255	LYS	N-CA-C	6.41	118.83	111.02
1	B	51	SER	N-CA-C	-6.40	102.77	110.13
1	A	249	LYS	CA-C-N	-6.05	112.28	119.84
1	A	249	LYS	C-N-CA	-6.05	112.28	119.84
1	A	73	LEU	N-CA-C	5.72	119.07	111.75
1	B	137	ASN	N-CA-C	5.58	118.81	109.95
1	B	127	TRP	N-CA-C	-5.49	105.22	111.14
1	B	247	ILE	N-CA-C	5.44	113.25	107.76
1	A	95	SER	N-CA-C	5.39	117.52	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	GLU	N-CA-C	-5.30	102.56	110.20
1	B	152	ILE	N-CA-C	5.18	120.12	109.34
1	B	351	ASP	N-CA-C	-5.15	105.74	112.23
1	B	259	GLU	N-CA-C	-5.14	105.75	112.23
1	A	72	PRO	N-CA-C	-5.13	103.05	111.21
1	B	289	GLY	N-CA-C	-5.03	102.39	111.19
1	B	71	LEU	N-CA-C	5.02	116.88	109.50

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	167	0
1	B	2710	0	2782	135	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	292	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 26.

All (292) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:A:249:LYS:HA	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:251:LEU:HD11	1:A:263:LYS:HZ3	1.59	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:38:LEU:HB3	1:A:45:LEU:HB2	1.78	0.65
1:A:314:LEU:HD21	1:A:320:VAL:CG1	2.26	0.65
1:B:255:LYS:HG3	1:B:256:SER:N	2.12	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:B:222:ARG:NH1	2.10	0.63
1:B:130:LEU:HA	4:B:518:HOH:O	1.97	0.63
1:A:77:ILE:HD11	1:A:108:ASN:CG	2.24	0.62
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:55:VAL:O	1:A:56:GLY:C	2.43	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:73:LEU:HD23	1:A:97:TYR:CE2	2.36	0.61
1:A:196:ASP:O	1:A:200:VAL:HG23	2.00	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:59:TRP:CH2	1:B:60:LYS:HE3	2.36	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: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: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
1:B:348:VAL:O	1:B:352:VAL:HG23	2.03	0.56
1:A:160:ILE:HD11	1:A:166:VAL:HG23	1.87	0.56
1:B:166:VAL:HG11	1:B:231:SER:HB3	1.87	0.56
1:A:21:LEU:HD11	1:A:38:LEU:HD11	1.88	0.56
1:A:185:SER:HB3	1:A:275:LYS:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:143:GLU:C	1:B:145:THR:H	2.15	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:141:TYR:HB3	1:B:351:ASP:OD2	2.07	0.54
1:B:212:ARG:HD2	1:B:260:PHE:CD1	2.42	0.54
1:A:7:ASN:ND2	1:A:34:ASN:HB2	2.22	0.54
1:A:127:TRP:HA	1:A:130:LEU:HD12	1.88	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:121:SER:OG	1:B:222:ARG:HD3	2.08	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND2	1:B:137:ASN:H	2.10	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:251:LEU:HD11	1:A:263:LYS:NZ	2.26	0.49
1:A:222:ARG:O	1:A:226:ILE:HG13	2.12	0.49
1:B:3:THR:HG21	1:B:32:THR:OG1	2.13	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: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:37:LEU:CD1	1:B:46:ILE:HG12	2.43	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: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:HG3	1:A:157:ARG:HH11	1.77	0.48
1:A:302:ILE:HG22	1:A:303:GLU:N	2.27	0.48
1:A:50:PHE:CE2	1:A:83:SER:HB2	2.48	0.48
1:A:176:THR:O	1:A:180:ILE:HG13	2.13	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
1:A:30:THR:HG22	1:A:30:THR:O	2.13	0.48
1:A:319:ASN:CG	1:A:338:GLY:HA3	2.38	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:250:PRO:O	1:A:251:LEU:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:SER:OG	1:B:97:TYR:HB3	2.14	0.47
1:B:143:GLU:C	1:B:145:THR:N	2.71	0.47
1:B:212:ARG:HG3	1:B:260:PHE:CZ	2.49	0.47
1:B:332:VAL:O	1:B:332:VAL:HG12	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:H	1:B:137:ASN:HD22	1.62	0.47
1:B:267:TYR:CD1	1:B:267:TYR:N	2.83	0.47
1:A:3:THR:O	1:A:31:ILE:HG12	2.14	0.47
1:A:152:ILE:HD12	1:A:321:ILE:CD1	2.45	0.47
1:B:58:ASP:OD2	1:B:60:LYS:HB2	2.13	0.47
1:B:121:SER:OG	1:B:222:ARG:CD	2.63	0.47
1:A:302:ILE:CG2	1:A:303:GLU:N	2.78	0.47
1:B:148:ALA:HB2	1:B:338:GLY:C	2.39	0.47
1:B:134:LYS:HB2	1:B:137:ASN:CG	2.40	0.47
1:A:315:LYS:O	1:A:316:GLY:C	2.56	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:HD22	1:A:330:ASN:HA	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:B:276:LYS:O	1:B:277:GLU:C	2.59	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:256:SER:O	1:A:257:ALA:C	2.59	0.46
1:A:180:ILE:HG23	1:A:197:VAL:CG1	2.46	0.45
1:A:208:GLU:O	1:A:209:PRO:C	2.57	0.45
1:A:334:ILE:HG23	1:B:334:ILE:HD13	1.97	0.45
1:A:101:PHE:O	1:A:102:TYR:C	2.60	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:59:TRP:CD1	1:A:59:TRP:H	2.35	0.45
1:A:73:LEU:O	1:A:77:ILE:CG2	2.64	0.45
1:A:221:ALA:HA	1:A:224:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:132:SER:C	1:B:134:LYS:N	2.74	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:A:237:SER:C	1:A:239:THR:H	2.25	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:332:VAL:O	1:B:333:VAL:C	2.58	0.44
1:B:349:LEU:O	1:B:352:VAL:HB	2.18	0.44
1:B:270:ASP:OD2	1:B:270:ASP:N	2.45	0.44
1:A:208:GLU:HG2	1:A:214:ASP:OD2	2.18	0.44
1:B:132:SER:C	1:B:134:LYS:H	2.25	0.43
1:A:248:PRO:O	1:A:249:LYS:C	2.61	0.43
1:B:83:SER:HA	1:B:84:PRO:HD3	1.83	0.43
1:B:330:ASN:HB2	4:B:507:HOH:O	2.18	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:276:LYS:O	1:A:279:ALA:HB3	2.18	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:63:LEU:O	1:A:66:SER:HB3	2.18	0.43
1:A:267:TYR:CD2	1:A:267:TYR:N	2.86	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:10:VAL:HG22	1:A:90:VAL:HB	2.01	0.43
1:A:264:LEU:C	1:A:266:ASP:H	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:163:GLY:C	1:B:327:ARG:HH21	2.27	0.42
1:B:314:LEU:HD11	1:B:320:VAL:CG2	2.48	0.42
1:A:157:ARG:HG3	1:A:157:ARG:NH1	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:A:52:PRO:O	1:A:53:LEU:C	2.63	0.41
1:B:266:ASP:C	1:B:267:TYR:CD1	2.99	0.41
1:A:24:LEU:C	1:A:24:LEU:CD2	2.94	0.41
1:A:202:LYS:HD2	1:A:261:LEU:HD11	2.02	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:B:20:PHE:CD2	1:B:20:PHE:C	2.98	0.41
1:B:212:ARG:O	1:B:247:ILE:HD11	2.19	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:319:ASN:O	1:A:335:GLN:HA	2.21	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:B:208:GLU:O	1:B:209:PRO:C	2.64	0.41
1:B:248:PRO:O	1:B:249:LYS:C	2.63	0.41
1:A:73:LEU:O	1:A:77:ILE:HG22	2.20	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:179:TYR:HB2	1:A:317:SER:HB3	2.03	0.40
1:A:237:SER:C	1:A:239:THR:N	2.78	0.40
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.97	0.40
1:A:89:LEU:HD22	1:A:105:PHE:CD2	2.56	0.40
1:A:181:PHE:HE1	1:A:246:LEU:HD21	1.85	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: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%)	6	12
1	B	356/359 (99%)	315 (88%)	34 (10%)	7 (2%)	6	12
All	All	712/718 (99%)	628 (88%)	70 (10%)	14 (2%)	6	12

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%)	22	46
1	B	300/301 (100%)	284 (95%)	16 (5%)	20	43
All	All	600/602 (100%)	569 (95%)	31 (5%)	21	44

All (31) 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	248	PRO
1	A	250	PRO
1	A	330	ASN
1	B	71	LEU
1	B	80	LEU
1	B	137	ASN
1	B	145	THR
1	B	162	THR
1	B	187	SER
1	B	198	VAL
1	B	209	PRO
1	B	215	LEU
1	B	220	VAL
1	B	222	ARG
1	B	270	ASP
1	B	284	VAL
1	B	300	VAL
1	B	320	VAL
1	B	326	LYS

Sometimes 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	108	ASN
1	A	133	ASN
1	A	142	HIS
1	A	161	GLN
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	282	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 oligosaccharides 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]	-	54,58,58	2.99	8 (14%)	70,88,88	1.91	16 (22%)
3	NHO	A	361[B]	-	54,58,58	2.99	8 (14%)	70,88,88	1.92	16 (22%)

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[B]	-	1/1/15/15	16/46/78/78	0/5/5/5
3	NHO	A	361[A]	-	-	16/46/78/78	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361[A]	NHO	C3N-C4N	15.58	1.57	1.40
3	A	361[B]	NHO	C3N-C4N	15.45	1.57	1.40
3	A	361[B]	NHO	C5N-C4N	11.31	1.53	1.39
3	A	361[A]	NHO	C5N-C4N	11.19	1.53	1.39
3	A	361[B]	NHO	C2N-N1N	6.30	1.41	1.35
3	A	361[A]	NHO	C2N-N1N	6.20	1.41	1.35
3	A	361[A]	NHO	C4N-C5R	3.89	1.58	1.52
3	A	361[B]	NHO	C4N-C5R	3.85	1.58	1.52
3	A	361[A]	NHO	C6N-N1N	3.24	1.42	1.35
3	A	361[B]	NHO	C6N-N1N	3.20	1.42	1.35
3	A	361[A]	NHO	C4A-N3A	3.11	1.40	1.34
3	A	361[B]	NHO	C4A-N3A	3.09	1.40	1.34
3	A	361[B]	NHO	C2A-N1A	2.54	1.38	1.33
3	A	361[A]	NHO	C2A-N1A	2.53	1.38	1.33
3	A	361[A]	NHO	PA-OPP	2.03	1.61	1.59
3	A	361[B]	NHO	PA-OPP	2.01	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361[B]	NHO	C5N-C4N-C5R	-5.44	108.44	120.21
3	A	361[A]	NHO	C5N-C4N-C5R	-5.37	108.59	120.21
3	A	361[B]	NHO	C4A-N9A-C8A	5.22	111.22	105.74
3	A	361[A]	NHO	C4A-N9A-C8A	5.21	111.21	105.74
3	A	361[B]	NHO	N3A-C4A-N9A	5.20	136.01	127.17
3	A	361[A]	NHO	N3A-C4A-N9A	5.17	135.96	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361[A]	NHO	C5N-C4N-C3N	-5.10	112.77	118.78
3	A	361[B]	NHO	C5N-C4N-C3N	-5.09	112.78	118.78
3	A	361[B]	NHO	O1A-PA-OPP	3.94	117.91	107.27
3	A	361[A]	NHO	O1A-PA-OPP	3.93	117.90	107.27
3	A	361[B]	NHO	C5A-C4A-N9A	-3.73	101.74	105.81
3	A	361[A]	NHO	C5A-C4A-N9A	-3.67	101.81	105.81
3	A	361[B]	NHO	O4'-C1'-N9A	3.39	114.59	108.09
3	A	361[A]	NHO	O4'-C1'-N9A	3.38	114.58	108.09
3	A	361[A]	NHO	C5A-C4A-N3A	-3.26	122.23	126.72
3	A	361[B]	NHO	C5A-C4A-N3A	-3.24	122.25	126.72
3	A	361[B]	NHO	O7N-C7N-C3N	-3.03	116.67	120.24
3	A	361[A]	NHO	N9A-C8A-N7A	-3.00	109.68	113.94
3	A	361[A]	NHO	O7N-C7N-C3N	-3.00	116.70	120.24
3	A	361[B]	NHO	N9A-C8A-N7A	-2.96	109.74	113.94
3	A	361[B]	NHO	C6N-N1N-C2N	2.65	124.13	121.88
3	A	361[B]	NHO	C4'-O4'-C1'	-2.64	103.64	109.47
3	A	361[A]	NHO	C4'-O4'-C1'	-2.62	103.69	109.47
3	A	361[A]	NHO	C6N-N1N-C2N	2.57	124.07	121.88
3	A	361[B]	NHO	OPP-PA-O2A	-2.57	102.98	110.70
3	A	361[A]	NHO	OPP-PA-O2A	-2.56	103.02	110.70
3	A	361[B]	NHO	C3N-C2N-N1N	-2.41	118.69	122.58
3	A	361[A]	NHO	C3N-C2N-N1N	-2.39	118.72	122.58
3	A	361[A]	NHO	N6A-C6A-N1A	2.34	123.59	118.38
3	A	361[B]	NHO	N6A-C6A-N1A	2.32	123.55	118.38
3	A	361[B]	NHO	C5A-C6A-N6A	-2.10	118.10	123.29
3	A	361[A]	NHO	C5A-C6A-N6A	-2.09	118.11	123.29

All (1) chirality outliers are listed below:

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

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	361[A]	NHO	C5'-O5'-PA-OPP
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	C5'-O5'-PA-OPP
3	A	361[B]	NHO	C5N-C4N-C5R-O5R

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Mol	Chain	Res	Type	Atoms
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-C4N
3	A	361[B]	NHO	O4R-C4R-C5R-C4N
3	A	361[A]	NHO	C4N-C3N-C7N-O7N
3	A	361[B]	NHO	C4N-C3N-C7N-O7N
3	A	361[A]	NHO	C5N-C4N-C5R-C4R
3	A	361[B]	NHO	C5N-C4N-C5R-C4R
3	A	361[A]	NHO	PN-OPP-PA-O2A
3	A	361[B]	NHO	PN-OPP-PA-O2A
3	A	361[A]	NHO	C2R-C3R-C4R-C5R
3	A	361[B]	NHO	C2R-C3R-C4R-C5R
3	A	361[A]	NHO	O1R-C1R-C2R-C3R
3	A	361[B]	NHO	O1R-C1R-C2R-C3R
3	A	361[A]	NHO	C3R-C4R-C5R-C4N
3	A	361[B]	NHO	C3R-C4R-C5R-C4N
3	A	361[A]	NHO	OR-C1R-C2R-C3R
3	A	361[B]	NHO	OR-C1R-C2R-C3R
3	A	361[A]	NHO	O4B-C1B-N1N-C2N
3	A	361[A]	NHO	O4B-C1B-N1N-C6N
3	A	361[B]	NHO	O4B-C1B-N1N-C2N
3	A	361[B]	NHO	O4B-C1B-N1N-C6N
3	A	361[A]	NHO	C4N-C3N-C7N-N7N
3	A	361[B]	NHO	C4N-C3N-C7N-N7N

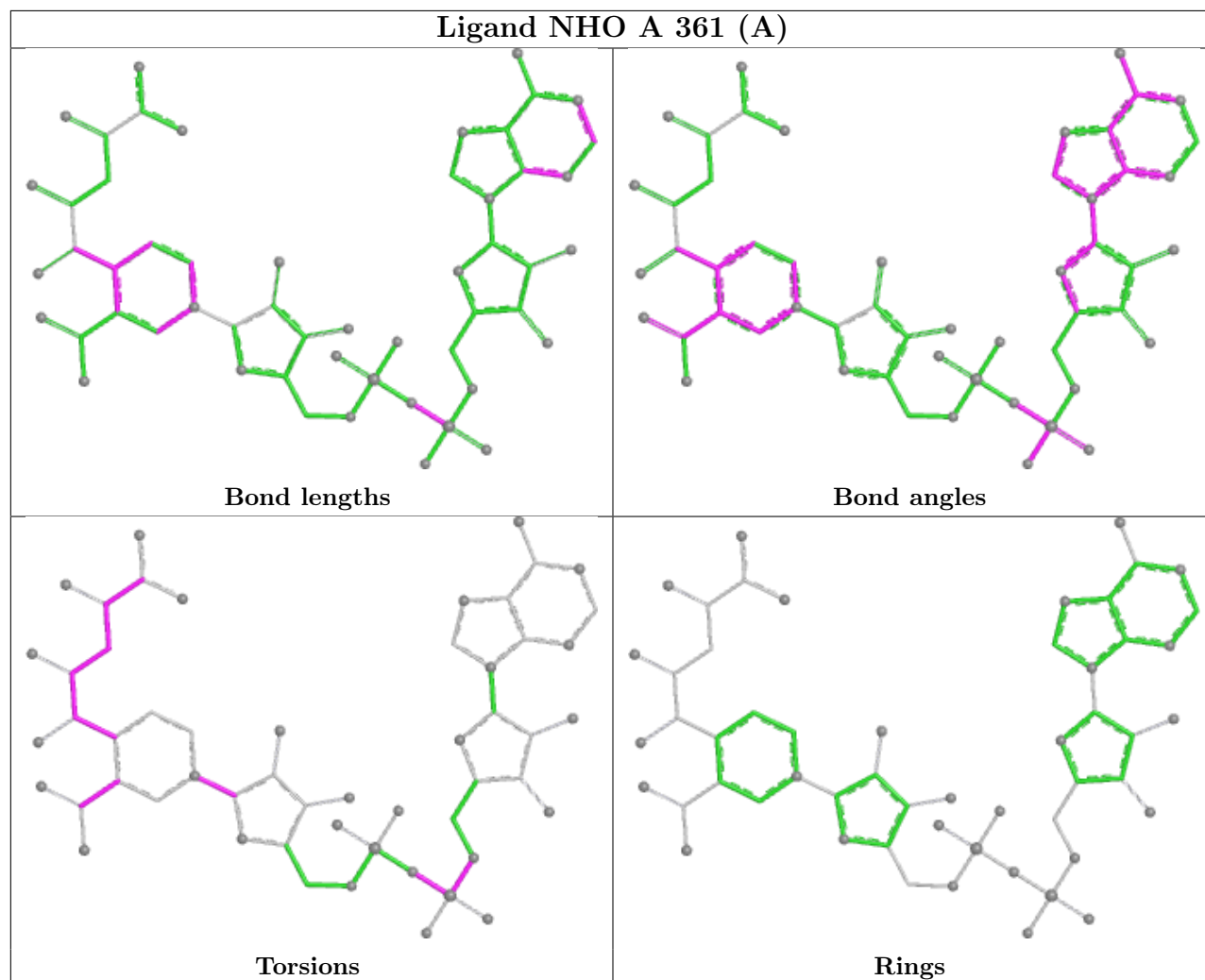
There are no ring outliers.

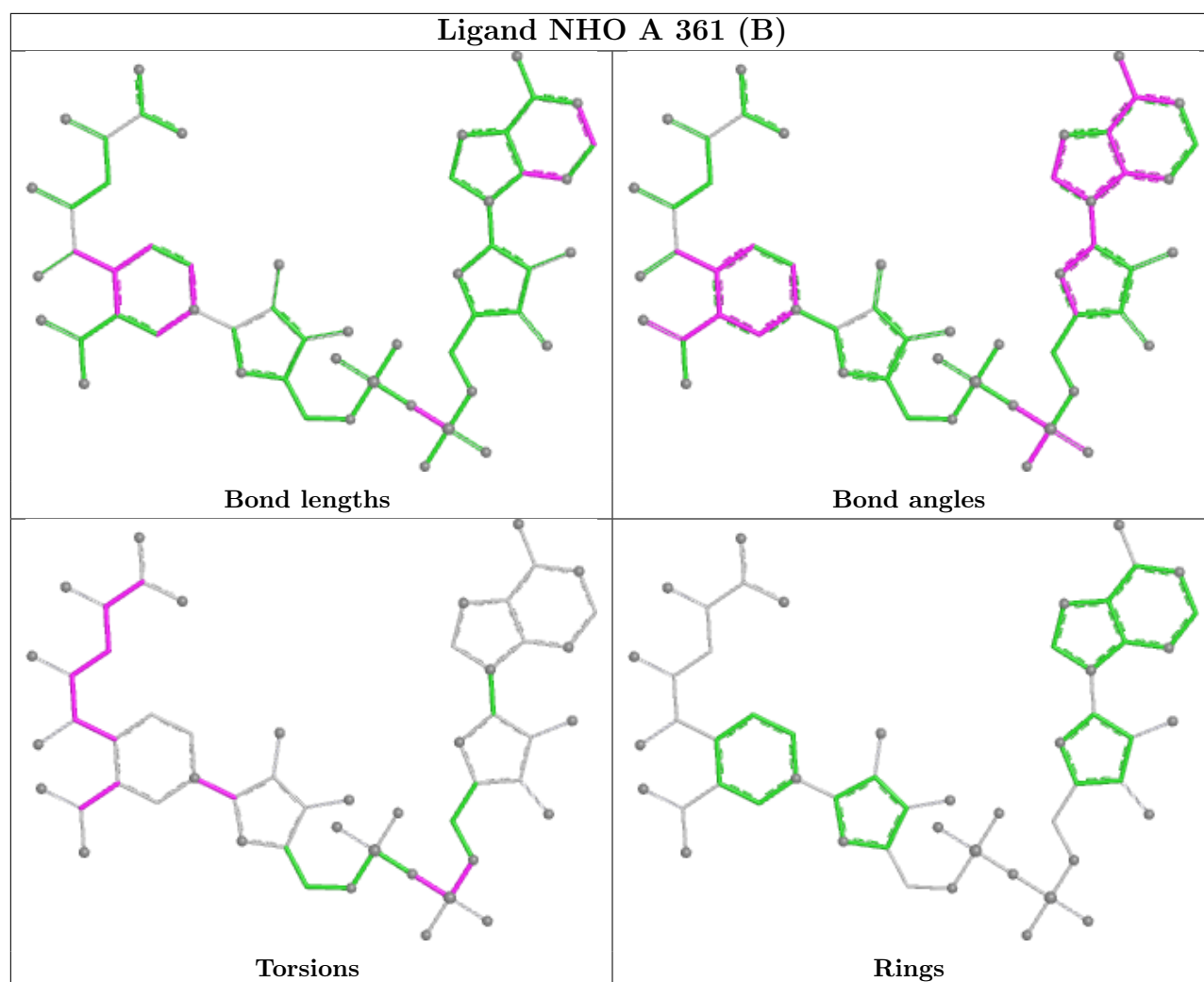
2 monomers are involved in 2 short contacts:

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.





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%)	0.33	30 (8%) 17 13	11, 29, 76, 89	0
1	B	358/359 (99%)	0.09	12 (3%) 48 42	13, 29, 46, 70	0
All	All	716/718 (99%)	0.21	42 (5%) 28 23	11, 29, 69, 89	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	VAL	6.3
1	A	3	THR	6.0
1	A	251	LEU	5.1
1	B	132	SER	4.9
1	A	2	SER	4.8
1	B	130	LEU	3.7
1	A	249	LYS	3.7
1	B	136	THR	3.6
1	A	263	LYS	3.5
1	A	257	ALA	3.5
1	B	131	PHE	3.4
1	A	267	TYR	3.4
1	A	255	LYS	3.3
1	A	250	PRO	3.2
1	A	261	LEU	3.1
1	A	262	GLU	3.1
1	A	256	SER	3.1
1	A	56	GLY	3.0
1	B	263	LYS	2.8
1	B	189	ALA	2.8
1	A	58	ASP	2.7
1	A	187	SER	2.7
1	A	55	VAL	2.7
1	A	248	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2	SER	2.6
1	A	281	GLU	2.6
1	A	253	SER	2.5
1	A	190	ASN	2.4
1	A	259	GLU	2.4
1	B	137	ASN	2.3
1	B	135	PRO	2.3
1	B	294	ALA	2.3
1	A	271	LEU	2.3
1	A	206	TYR	2.3
1	A	306	ASP	2.3
1	B	187	SER	2.2
1	A	191	ASP	2.1
1	B	64	ALA	2.1
1	A	308	SER	2.1
1	A	269	LYS	2.1
1	A	284	VAL	2.0
1	A	264	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

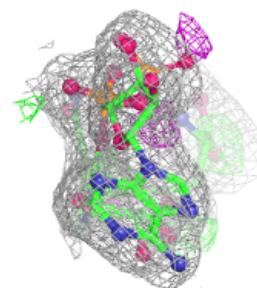
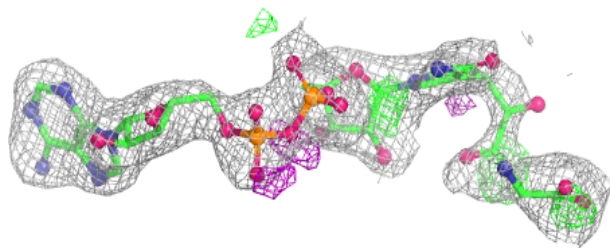
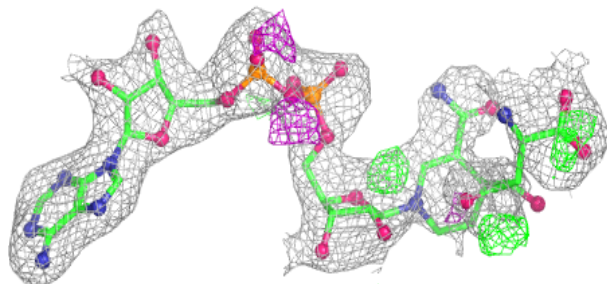
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NHO	A	361[A]	54/54	0.87	0.14	22,40,55,55	54
3	NHO	A	361[B]	54/54	0.87	0.14	22,40,55,55	54
2	NA	A	500	1/1	0.94	0.07	25,25,25,25	0
2	NA	B	501	1/1	0.94	0.07	34,34,34,34	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.

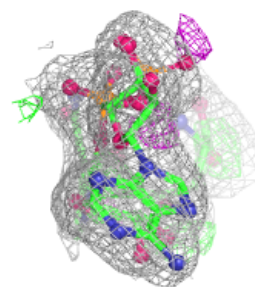
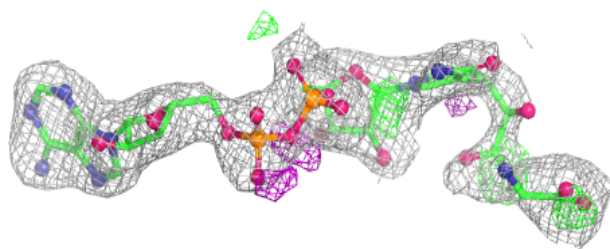
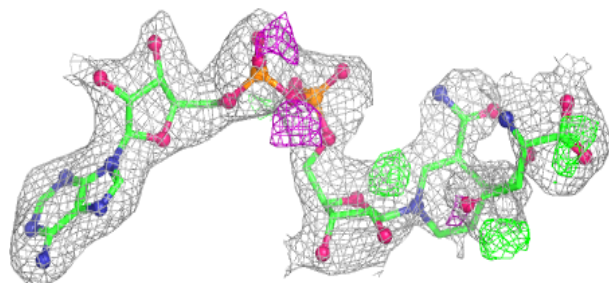
Electron density around NHO A 361 (A):

$2mF_o-DF_c$ (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 (B):

$2mF_o-DF_c$ (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.