



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 PM UTC

PDB ID : 1NUO / pdb_00001nuo
Title : Two RTH Mutants with Impaired Hormone Binding
Authors : Huber, B.R.; Sandler, B.; West, B.L.; Cunha-Lima, S.T.; Nguyen, H.T.;
Apriletti, J.W.; Baxter, J.D.; Fletterick, R.J.
Deposited on : 2003-01-31
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

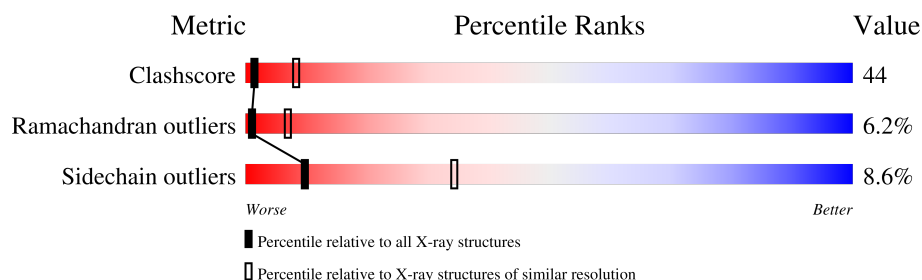
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	21% 42% 28% • 5%

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
2	4HY	A	500	-	X	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1908 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.

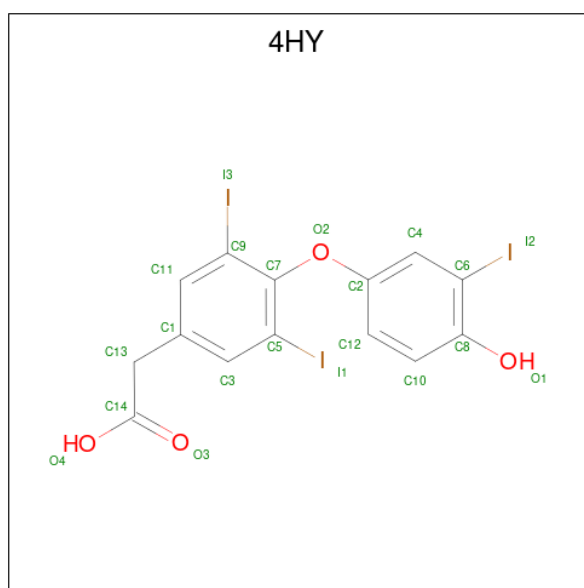
- Molecule 1 is a protein called Thyroid hormone receptor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	1887	1216	314	340	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ASP	GLU	conflict	UNP P10828
A	316	HIS	ARG	variant	UNP P10828

- Molecule 2 is [4-(4-HYDROXY-3-iodo-PHENOXY)-3,5-DIIODO-PHENYL]-ACETIC ACID (CCD ID: 4HY) (formula: C₁₄H₉I₃O₄).



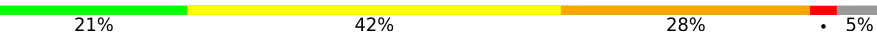
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	I	O		
2	A	1	21	14	3	4	0	0

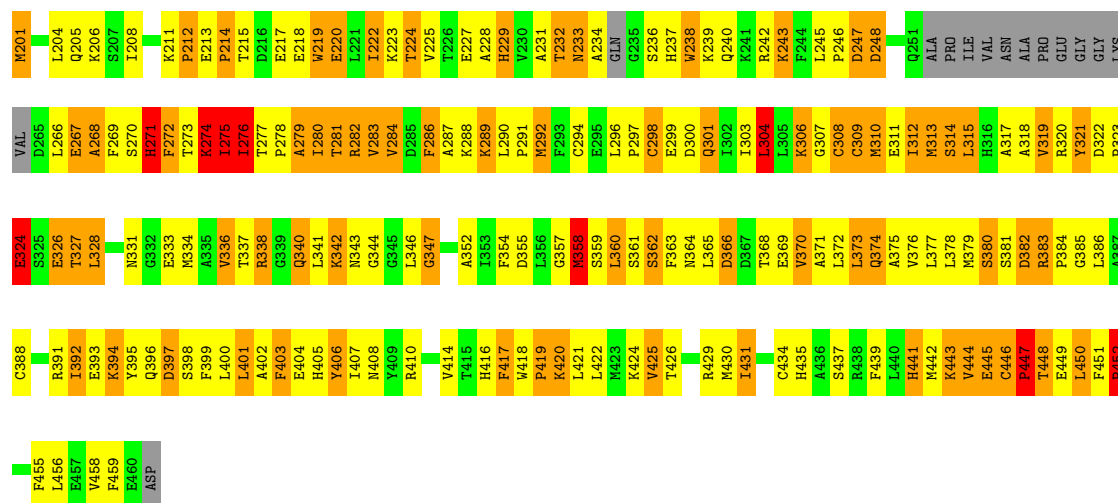
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Thyroid hormone receptor beta-1

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.27 Å 67.27 Å 130.12 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	96.7 (20.00-3.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.252 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1908	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HY

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	2.61	121/1930 (6.3%)	1.79	46/2621 (1.8%)

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	CYS	C-O	-14.32	1.07	1.24
1	A	233	ASN	CA-C	11.90	1.68	1.52
1	A	222	ILE	C-O	-10.72	1.11	1.24
1	A	319	VAL	CA-CB	-10.29	1.40	1.54
1	A	314	SER	C-O	10.13	1.35	1.24
1	A	371	ALA	CA-C	-9.79	1.40	1.52
1	A	282	ARG	CA-CB	9.65	1.68	1.53
1	A	289	LYS	C-O	9.22	1.35	1.24
1	A	283	VAL	C-O	-9.10	1.14	1.24
1	A	417	PHE	C-O	-9.05	1.13	1.24
1	A	340	GLN	C-O	-8.99	1.13	1.24
1	A	222	ILE	CA-CB	-8.82	1.43	1.54
1	A	268	ALA	C-O	-8.50	1.14	1.24
1	A	398	SER	C-O	-8.43	1.14	1.24
1	A	303	ILE	CA-CB	-8.42	1.45	1.54
1	A	336	VAL	CA-C	-8.34	1.42	1.52
1	A	364	ASN	C-O	-8.02	1.13	1.23
1	A	233	ASN	C-O	7.98	1.34	1.24
1	A	375	ALA	C-O	-7.96	1.14	1.24
1	A	328	LEU	C-O	-7.86	1.14	1.23
1	A	447	PRO	CA-C	7.85	1.63	1.52
1	A	397	ASP	N-CA	-7.78	1.36	1.46
1	A	279	ALA	CA-CB	-7.78	1.41	1.53
1	A	368	THR	CA-C	-7.77	1.42	1.52
1	A	281	THR	CA-C	7.56	1.62	1.52
1	A	393	GLU	C-O	-7.55	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	C-O	-7.48	1.14	1.24
1	A	288	LYS	C-O	7.43	1.32	1.24
1	A	441	HIS	CA-C	7.38	1.63	1.52
1	A	232	THR	C-O	-7.27	1.16	1.24
1	A	308	CYS	C-O	-7.25	1.14	1.24
1	A	379	MET	CA-C	-7.24	1.43	1.53
1	A	340	GLN	CA-C	-7.19	1.43	1.52
1	A	434	CYS	CA-C	-7.18	1.43	1.52
1	A	298	CYS	CA-C	-7.08	1.43	1.52
1	A	355	ASP	C-O	-7.08	1.15	1.24
1	A	406	TYR	C-O	-7.02	1.15	1.24
1	A	276	ILE	C-O	-6.99	1.17	1.24
1	A	213	GLU	C-O	-6.99	1.13	1.23
1	A	289	LYS	CA-C	6.97	1.62	1.52
1	A	292	MET	C-O	-6.86	1.16	1.24
1	A	301	GLN	C-O	-6.84	1.16	1.24
1	A	422	LEU	C-O	6.79	1.32	1.24
1	A	275	ILE	C-O	-6.75	1.16	1.24
1	A	243	LYS	C-O	-6.70	1.15	1.24
1	A	425	VAL	CA-C	-6.66	1.43	1.52
1	A	298	CYS	CA-CB	6.66	1.63	1.53
1	A	434	CYS	N-CA	-6.65	1.38	1.46
1	A	275	ILE	CA-C	-6.59	1.44	1.52
1	A	452	PRO	C-O	-6.58	1.17	1.24
1	A	337	THR	CA-C	6.57	1.62	1.53
1	A	384	PRO	CA-C	-6.55	1.44	1.52
1	A	431	ILE	CA-CB	-6.51	1.46	1.54
1	A	310	MET	SD-CE	6.49	1.95	1.79
1	A	398	SER	CA-C	-6.39	1.44	1.52
1	A	420	LYS	N-CA	-6.37	1.38	1.46
1	A	336	VAL	C-O	-6.37	1.16	1.23
1	A	212	PRO	CA-C	6.29	1.61	1.52
1	A	271	HIS	C-O	6.24	1.31	1.24
1	A	284	VAL	CA-CB	-6.20	1.47	1.54
1	A	382	ASP	CB-CG	6.17	1.67	1.52
1	A	352	ALA	CA-CB	-6.12	1.43	1.53
1	A	217	GLU	CA-C	6.08	1.61	1.52
1	A	419	PRO	C-O	-6.08	1.16	1.24
1	A	374	GLN	CA-C	-6.05	1.44	1.52
1	A	336	VAL	CA-CB	-6.04	1.44	1.54
1	A	406	TYR	CA-C	-6.02	1.44	1.52
1	A	224	THR	CA-C	-6.01	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	LYS	CA-C	-6.00	1.45	1.52
1	A	418	TRP	C-O	-5.95	1.18	1.24
1	A	358	MET	SD-CE	-5.90	1.64	1.79
1	A	426	THR	N-CA	5.89	1.53	1.46
1	A	236	SER	CA-C	5.86	1.60	1.52
1	A	347	GLY	C-O	-5.84	1.15	1.24
1	A	306	LYS	C-O	5.83	1.30	1.24
1	A	321	TYR	N-CA	5.82	1.53	1.46
1	A	280	ILE	CA-C	-5.81	1.44	1.52
1	A	326	GLU	CA-C	-5.77	1.45	1.53
1	A	211	LYS	CA-CB	-5.76	1.46	1.53
1	A	360	LEU	C-O	-5.73	1.16	1.24
1	A	287	ALA	CA-C	-5.73	1.45	1.52
1	A	274	LYS	C-O	5.72	1.31	1.24
1	A	383	ARG	CG-CD	-5.66	1.35	1.52
1	A	370	VAL	CA-C	5.64	1.60	1.52
1	A	238	TRP	N-CA	5.63	1.53	1.46
1	A	272	PHE	C-O	-5.60	1.17	1.24
1	A	301	GLN	CA-C	-5.60	1.45	1.52
1	A	309	CYS	C-O	-5.58	1.17	1.24
1	A	220	GLU	C-O	5.56	1.30	1.24
1	A	274	LYS	CA-CB	5.56	1.62	1.53
1	A	239	LYS	CA-C	-5.56	1.44	1.52
1	A	292	MET	CG-SD	5.54	1.94	1.80
1	A	215	THR	N-CA	-5.54	1.38	1.45
1	A	227	GLU	CA-CB	-5.50	1.44	1.53
1	A	373	LEU	CA-C	5.47	1.59	1.52
1	A	223	LYS	C-O	5.44	1.30	1.24
1	A	286	PHE	C-O	-5.43	1.17	1.24
1	A	231	ALA	CA-CB	5.41	1.62	1.53
1	A	338	ARG	C-O	5.38	1.30	1.24
1	A	214	PRO	CA-C	-5.38	1.46	1.52
1	A	298	CYS	CB-SG	5.37	1.99	1.81
1	A	434	CYS	C-N	-5.35	1.26	1.34
1	A	237	HIS	N-CA	-5.31	1.41	1.46
1	A	366	ASP	CA-C	-5.28	1.46	1.52
1	A	288	LYS	CA-C	5.25	1.59	1.52
1	A	426	THR	CA-CB	-5.22	1.45	1.53
1	A	437	SER	C-O	-5.20	1.17	1.24
1	A	213	GLU	CA-CB	-5.17	1.45	1.53
1	A	402	ALA	N-CA	-5.15	1.39	1.46
1	A	417	PHE	CE1-CZ	-5.13	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	ASP	C-O	-5.12	1.17	1.24
1	A	309	CYS	CA-C	-5.12	1.46	1.52
1	A	382	ASP	CG-OD1	5.08	1.35	1.25
1	A	313	MET	SD-CE	-5.08	1.66	1.79
1	A	414	VAL	C-O	-5.08	1.18	1.24
1	A	279	ALA	C-N	-5.07	1.27	1.33
1	A	304	LEU	N-CA	-5.05	1.40	1.46
1	A	380	SER	CA-C	5.04	1.59	1.52
1	A	281	THR	C-O	-5.03	1.18	1.24
1	A	308	CYS	CA-C	-5.02	1.45	1.52
1	A	222	ILE	C-N	-5.01	1.27	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	LYS	N-CA-C	-9.08	101.97	112.87
1	A	424	LYS	N-CA-C	-7.80	103.02	112.54
1	A	229	HIS	N-CA-C	-7.70	101.86	111.11
1	A	224	THR	CA-C-O	-7.18	113.22	120.90
1	A	362	SER	N-CA-C	-7.11	105.80	114.75
1	A	447	PRO	N-CA-C	7.10	127.09	112.47
1	A	296	LEU	CA-C-N	6.95	127.89	120.11
1	A	296	LEU	C-N-CA	6.95	127.89	120.11
1	A	394	LYS	CA-C-O	6.66	127.61	120.55
1	A	306	LYS	CA-C-O	6.61	127.51	120.70
1	A	220	GLU	CA-C-N	6.59	129.41	120.38
1	A	220	GLU	C-N-CA	6.59	129.41	120.38
1	A	326	GLU	CA-C-O	-6.57	114.22	121.84
1	A	292	MET	CA-C-O	6.20	126.99	120.42
1	A	431	ILE	N-CA-C	-6.10	104.40	110.62
1	A	380	SER	N-CA-C	6.01	117.99	108.67
1	A	309	CYS	N-CA-C	6.01	118.35	111.02
1	A	392	ILE	N-CA-C	-5.96	104.22	112.50
1	A	401	LEU	CA-C-O	5.92	126.83	120.55
1	A	447	PRO	N-CD-CG	-5.80	94.50	103.20
1	A	233	ASN	CA-C-O	5.72	128.70	120.51
1	A	452	PRO	N-CA-C	5.72	117.67	110.70
1	A	298	CYS	CA-CB-SG	5.68	127.46	114.40
1	A	403	PHE	CA-C-O	5.66	126.53	120.70
1	A	219	TRP	N-CA-C	-5.56	105.59	112.38
1	A	298	CYS	O-C-N	5.55	128.01	122.12
1	A	425	VAL	N-CA-C	-5.55	104.16	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LEU	CA-C-O	-5.54	114.93	120.63
1	A	315	LEU	N-CA-C	-5.53	105.15	111.07
1	A	450	LEU	N-CA-C	5.53	122.58	110.80
1	A	267	GLU	N-CA-C	-5.48	104.17	111.24
1	A	402	ALA	N-CA-C	-5.47	105.48	111.82
1	A	232	THR	CA-C-O	-5.44	113.37	119.08
1	A	298	CYS	N-CA-C	-5.40	105.40	111.28
1	A	326	GLU	CB-CA-C	-5.37	104.26	111.89
1	A	289	LYS	CA-C-O	5.36	126.16	120.10
1	A	314	SER	O-C-N	5.34	127.86	122.09
1	A	224	THR	O-C-N	5.34	127.64	122.09
1	A	394	LYS	O-C-N	-5.25	116.55	122.12
1	A	382	ASP	CB-CG-OD1	5.25	130.47	118.40
1	A	441	HIS	N-CA-C	-5.22	106.01	112.38
1	A	268	ALA	O-C-N	-5.21	116.60	122.12
1	A	394	LYS	N-CA-C	-5.19	105.63	111.28
1	A	268	ALA	N-CA-C	-5.16	105.65	111.28
1	A	318	ALA	N-CA-C	5.05	117.68	111.82
1	A	323	PRO	N-CD-CG	-5.00	95.69	103.20

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	1887	0	1817	163	0
2	A	21	0	7	8	0
All	All	1908	0	1824	163	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 44.

All (163) 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:276:ILE:HG12	2:A:500:4HY:I1	2.01	1.31
1:A:276:ILE:CD1	2:A:500:4HY:I1	2.58	1.22
1:A:276:ILE:HD11	2:A:500:4HY:I1	2.12	1.19
1:A:276:ILE:CG1	2:A:500:4HY:I1	2.67	1.13
1:A:388:CYS:SG	1:A:391:ARG:NH2	2.30	1.05
1:A:416:HIS:O	1:A:419:PRO:HD2	1.64	0.97
1:A:444:VAL:HG23	1:A:445:GLU:N	1.84	0.92
1:A:444:VAL:HG23	1:A:445:GLU:H	1.35	0.91
1:A:201:MET:O	1:A:201:MET:HG3	1.68	0.90
1:A:267:GLU:O	1:A:270:SER:HB3	1.71	0.88
1:A:245:LEU:HD11	1:A:271:HIS:ND1	1.89	0.88
1:A:214:PRO:HB2	1:A:219:TRP:NE1	1.87	0.88
1:A:212:PRO:O	1:A:408:ASN:ND2	2.15	0.80
1:A:201:MET:O	1:A:201:MET:CG	2.32	0.76
1:A:214:PRO:HB2	1:A:219:TRP:CD1	2.19	0.76
1:A:280:ILE:O	1:A:284:VAL:HG23	1.84	0.75
1:A:370:VAL:O	1:A:374:GLN:HG3	1.86	0.74
1:A:242:ARG:HA	1:A:333:GLU:O	1.87	0.74
1:A:247:ASP:OD1	1:A:247:ASP:C	2.30	0.74
1:A:307:GLY:HA3	1:A:383:ARG:HD2	1.70	0.73
1:A:271:HIS:HB3	1:A:334:MET:HE1	1.71	0.72
1:A:416:HIS:C	1:A:419:PRO:HD2	2.13	0.72
1:A:297:PRO:O	1:A:301:GLN:HG3	1.90	0.71
1:A:416:HIS:O	1:A:417:PHE:C	2.35	0.70
1:A:439:PHE:CE2	1:A:443:LYS:HE3	2.26	0.70
1:A:277:THR:N	1:A:278:PRO:HD2	2.07	0.69
1:A:388:CYS:SG	1:A:391:ARG:CZ	2.80	0.69
1:A:276:ILE:HD13	2:A:500:4HY:I1	2.62	0.68
1:A:360:LEU:O	1:A:362:SER:N	2.27	0.67
1:A:342:LYS:HG3	1:A:347:GLY:HA2	1.77	0.66
1:A:309:CYS:SG	1:A:313:MET:HE2	2.35	0.66
1:A:360:LEU:C	1:A:362:SER:H	2.04	0.66
1:A:388:CYS:SG	1:A:391:ARG:NH1	2.70	0.65
1:A:276:ILE:HD11	2:A:500:4HY:C5	2.25	0.65
1:A:430:MET:HE3	1:A:430:MET:HA	1.78	0.65
1:A:225:VAL:HG21	1:A:399:PHE:HE2	1.60	0.64
1:A:445:GLU:O	1:A:446:CYS:SG	2.55	0.64
1:A:238:TRP:C	1:A:240:GLN:H	2.05	0.64
1:A:380:SER:HB2	1:A:383:ARG:HE	1.62	0.63
1:A:268:ALA:O	1:A:269:PHE:C	2.35	0.63
1:A:243:LYS:N	1:A:333:GLU:O	2.31	0.63
1:A:310:MET:O	1:A:314:SER:OG	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TRP:C	1:A:240:GLN:N	2.54	0.62
1:A:266:LEU:HD21	1:A:445:GLU:HG3	1.82	0.62
1:A:445:GLU:O	1:A:445:GLU:HG2	1.99	0.62
1:A:272:PHE:HE1	1:A:344:GLY:HA3	1.65	0.61
1:A:242:ARG:O	1:A:242:ARG:HG3	1.99	0.61
1:A:331:ASN:O	1:A:331:ASN:CG	2.42	0.61
1:A:286:PHE:CD1	1:A:286:PHE:C	2.78	0.61
1:A:317:ALA:O	1:A:328:LEU:HD22	2.00	0.61
1:A:447:PRO:O	1:A:448:THR:O	2.19	0.60
1:A:403:PHE:O	1:A:407:ILE:HG12	2.02	0.60
1:A:273:THR:CG2	1:A:452:PRO:HD3	2.31	0.59
1:A:429:ARG:HH11	1:A:429:ARG:HG2	1.67	0.59
1:A:444:VAL:C	1:A:446:CYS:H	2.10	0.59
1:A:341:LEU:HG	1:A:346:LEU:HD12	1.85	0.59
1:A:439:PHE:HA	1:A:442:MET:HE3	1.85	0.58
1:A:280:ILE:O	1:A:280:ILE:HG22	2.04	0.58
1:A:315:LEU:O	1:A:319:VAL:HG22	2.03	0.58
1:A:404:GLU:O	1:A:407:ILE:HB	2.03	0.57
1:A:444:VAL:C	1:A:446:CYS:N	2.62	0.57
1:A:214:PRO:HB2	1:A:219:TRP:CE2	2.39	0.57
1:A:271:HIS:O	1:A:272:PHE:C	2.48	0.56
1:A:286:PHE:CE1	1:A:290:LEU:HD11	2.40	0.56
1:A:233:ASN:O	1:A:234:ALA:C	2.48	0.56
1:A:245:LEU:HD11	1:A:271:HIS:CE1	2.42	0.55
1:A:446:CYS:SG	1:A:446:CYS:O	2.63	0.55
1:A:451:PHE:CD2	1:A:456:LEU:HD21	2.41	0.54
1:A:218:GLU:O	1:A:222:ILE:HG13	2.08	0.54
1:A:270:SER:O	1:A:273:THR:HB	2.07	0.54
1:A:425:VAL:O	1:A:429:ARG:HG3	2.08	0.54
1:A:444:VAL:CG2	1:A:445:GLU:N	2.59	0.54
1:A:273:THR:CG2	1:A:452:PRO:CD	2.86	0.53
1:A:416:HIS:O	1:A:419:PRO:CD	2.46	0.53
1:A:354:PHE:O	1:A:358:MET:HG2	2.08	0.53
1:A:441:HIS:O	1:A:444:VAL:HG22	2.09	0.53
1:A:280:ILE:O	1:A:280:ILE:CG2	2.56	0.53
1:A:228:ALA:O	1:A:229:HIS:C	2.52	0.52
1:A:245:LEU:HB3	1:A:340:GLN:HE22	1.74	0.52
1:A:342:LYS:O	1:A:344:GLY:N	2.43	0.52
1:A:246:PRO:O	1:A:247:ASP:C	2.51	0.51
1:A:240:GLN:NE2	1:A:240:GLN:HA	2.26	0.51
1:A:277:THR:N	1:A:278:PRO:CD	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASP:OD2	1:A:410:ARG:HD3	2.11	0.51
1:A:208:ILE:HG22	1:A:208:ILE:O	2.11	0.51
1:A:311:GLU:CD	1:A:383:ARG:HH22	2.20	0.50
1:A:275:ILE:HD13	1:A:334:MET:HE3	1.92	0.50
1:A:300:ASP:O	1:A:301:GLN:C	2.46	0.50
1:A:430:MET:O	1:A:431:ILE:C	2.52	0.50
1:A:442:MET:O	1:A:444:VAL:N	2.45	0.49
1:A:278:PRO:HG2	1:A:279:ALA:H	1.78	0.49
1:A:274:LYS:C	1:A:276:ILE:H	2.21	0.49
1:A:225:VAL:CG2	1:A:399:PHE:HE2	2.24	0.49
1:A:273:THR:HG23	1:A:452:PRO:CD	2.42	0.49
1:A:388:CYS:O	1:A:392:ILE:HG13	2.13	0.49
1:A:445:GLU:O	1:A:446:CYS:CB	2.59	0.49
1:A:273:THR:HG23	1:A:452:PRO:HD2	1.95	0.49
1:A:283:VAL:HG22	1:A:312:ILE:CG2	2.43	0.48
1:A:314:SER:O	1:A:317:ALA:HB3	2.13	0.48
1:A:357:GLY:O	1:A:358:MET:C	2.54	0.48
1:A:458:VAL:HG12	1:A:459:PHE:CD2	2.49	0.48
1:A:396:GLN:O	1:A:397:ASP:C	2.57	0.48
1:A:308:CYS:SG	1:A:312:ILE:HD13	2.54	0.48
1:A:247:ASP:OD1	1:A:248:ASP:N	2.46	0.48
1:A:267:GLU:O	1:A:270:SER:CB	2.55	0.47
1:A:275:ILE:O	1:A:275:ILE:HG13	2.14	0.47
1:A:304:LEU:HG	1:A:378:LEU:O	2.15	0.47
1:A:451:PHE:HD2	1:A:456:LEU:HD21	1.79	0.47
1:A:232:THR:HG23	1:A:289:LYS:HZ2	1.80	0.47
1:A:225:VAL:HG21	1:A:399:PHE:CE2	2.45	0.46
1:A:324:GLU:C	1:A:326:GLU:H	2.23	0.46
1:A:327:THR:HB	1:A:336:VAL:O	2.16	0.46
1:A:346:LEU:O	1:A:347:GLY:C	2.59	0.46
1:A:372:LEU:O	1:A:373:LEU:C	2.59	0.46
1:A:346:LEU:HD21	2:A:500:4HY:C8	2.45	0.46
1:A:272:PHE:HE2	1:A:336:VAL:HG11	1.81	0.46
1:A:360:LEU:C	1:A:362:SER:N	2.63	0.46
1:A:331:ASN:O	1:A:333:GLU:HG3	2.16	0.46
1:A:373:LEU:O	1:A:374:GLN:C	2.55	0.45
1:A:439:PHE:HE2	1:A:443:LYS:HE3	1.78	0.45
1:A:363:PHE:HD1	1:A:421:LEU:HD13	1.81	0.45
1:A:385:GLY:O	1:A:386:LEU:C	2.56	0.45
1:A:310:MET:HG2	1:A:435:HIS:CB	2.46	0.45
1:A:447:PRO:HB2	1:A:448:THR:H	1.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:O	1:A:282:ARG:C	2.59	0.45
1:A:369:GLU:O	1:A:370:VAL:C	2.57	0.45
1:A:406:TYR:CE2	1:A:410:ARG:HG3	2.52	0.45
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.50	0.44
1:A:443:LYS:O	1:A:447:PRO:HD3	2.17	0.44
1:A:319:VAL:HG23	1:A:320:ARG:N	2.33	0.44
1:A:366:ASP:OD1	1:A:369:GLU:HG3	2.16	0.44
1:A:341:LEU:CG	1:A:346:LEU:HD12	2.47	0.44
1:A:442:MET:C	1:A:444:VAL:N	2.73	0.44
1:A:313:MET:HB3	2:A:500:4HY:H131	2.00	0.44
1:A:451:PHE:HB3	1:A:456:LEU:HD21	2.00	0.44
1:A:394:LYS:O	1:A:395:TYR:C	2.57	0.44
1:A:417:PHE:CE2	1:A:421:LEU:HD22	2.53	0.44
1:A:286:PHE:CD1	1:A:286:PHE:O	2.71	0.43
1:A:365:LEU:HB3	1:A:369:GLU:HB2	1.99	0.43
1:A:429:ARG:HG2	1:A:429:ARG:NH1	2.32	0.43
1:A:276:ILE:C	1:A:278:PRO:HD2	2.42	0.43
1:A:271:HIS:O	1:A:274:LYS:N	2.52	0.43
1:A:376:VAL:O	1:A:377:LEU:C	2.60	0.43
1:A:357:GLY:O	1:A:359:SER:N	2.52	0.43
1:A:201:MET:O	1:A:205:GLN:HG3	2.19	0.42
1:A:267:GLU:O	1:A:270:SER:N	2.52	0.42
1:A:321:TYR:HB2	1:A:328:LEU:HD23	2.01	0.42
1:A:363:PHE:CD1	1:A:421:LEU:HD13	2.54	0.42
1:A:442:MET:O	1:A:443:LYS:C	2.61	0.42
1:A:292:MET:HE2	1:A:395:TYR:CD2	2.55	0.42
1:A:401:LEU:HD11	1:A:405:HIS:CE1	2.54	0.42
1:A:444:VAL:O	1:A:446:CYS:N	2.53	0.42
1:A:232:THR:HG23	1:A:289:LYS:NZ	2.34	0.41
1:A:306:LYS:O	1:A:307:GLY:C	2.61	0.41
1:A:204:LEU:C	1:A:206:LYS:N	2.79	0.41
1:A:407:ILE:HD13	1:A:407:ILE:HA	1.79	0.41
1:A:292:MET:SD	1:A:399:PHE:CE1	3.13	0.41
1:A:397:ASP:HA	1:A:400:LEU:HD12	2.02	0.41
1:A:338:ARG:HA	1:A:354:PHE:CE1	2.56	0.40
1:A:419:PRO:O	1:A:420:LYS:C	2.59	0.40
1:A:218:GLU:C	1:A:220:GLU:N	2.79	0.40
1:A:246:PRO:O	1:A:248:ASP:N	2.53	0.40
1:A:455:PHE:O	1:A:459:PHE:HD1	2.04	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	A	241/261 (92%)	193 (80%)	33 (14%)	15 (6%)	1 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ILE
1	A	444	VAL
1	A	447	PRO
1	A	448	THR
1	A	449	GLU
1	A	450	LEU
1	A	324	GLU
1	A	274	LYS
1	A	361	SER
1	A	443	LYS
1	A	342	LYS
1	A	271	HIS
1	A	343	ASN
1	A	452	PRO
1	A	446	CYS

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	A	197/229 (86%)	180 (91%)	17 (9%)	10 34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	MET
1	A	224	THR
1	A	247	ASP
1	A	248	ASP
1	A	276	ILE
1	A	294	CYS
1	A	298	CYS
1	A	299	GLU
1	A	304	LEU
1	A	312	ILE
1	A	324	GLU
1	A	327	THR
1	A	358	MET
1	A	381	SER
1	A	382	ASP
1	A	445	GLU
1	A	452	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	229	HIS
1	A	240	GLN
1	A	331	ASN
1	A	416	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	4HY	A	500	-	22,22,22	3.25	9 (40%)	31,31,31	3.18	18 (58%)

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	4HY	A	500	-	-	4/8/8/8	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	4HY	O1-C8	-8.60	1.19	1.36
2	A	500	4HY	C13-C14	-8.10	1.33	1.51
2	A	500	4HY	O4-C14	-6.26	1.10	1.30
2	A	500	4HY	C13-C1	2.81	1.56	1.51
2	A	500	4HY	C12-C10	2.67	1.43	1.38
2	A	500	4HY	C9-I3	-2.66	2.04	2.10
2	A	500	4HY	O2-C7	-2.61	1.34	1.39
2	A	500	4HY	C7-C5	2.20	1.46	1.40
2	A	500	4HY	C6-I2	-2.09	2.05	2.10

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	4HY	C13-C1-C3	7.18	131.28	120.38
2	A	500	4HY	C1-C13-C14	6.07	130.97	113.71
2	A	500	4HY	C10-C8-C6	-5.01	114.52	119.27
2	A	500	4HY	O3-C14-C13	4.85	137.57	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	4HY	C12-C2-C4	-4.58	114.35	120.50
2	A	500	4HY	O4-C14-O3	-4.39	112.03	123.33
2	A	500	4HY	C12-C10-C8	3.99	124.49	120.50
2	A	500	4HY	C2-C4-C6	3.94	126.89	119.14
2	A	500	4HY	C13-C1-C11	-3.74	114.71	120.38
2	A	500	4HY	C11-C1-C3	-3.68	114.00	119.01
2	A	500	4HY	O2-C7-C5	3.45	125.72	120.30
2	A	500	4HY	C8-C6-I2	3.06	122.71	119.76
2	A	500	4HY	O1-C8-C6	2.99	122.62	119.16
2	A	500	4HY	C1-C3-C5	2.85	125.67	120.45
2	A	500	4HY	C1-C11-C9	2.72	125.42	120.45
2	A	500	4HY	O2-C7-C9	-2.53	116.32	120.30
2	A	500	4HY	C11-C9-I3	2.03	122.28	118.46
2	A	500	4HY	O2-C2-C12	2.01	126.37	119.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

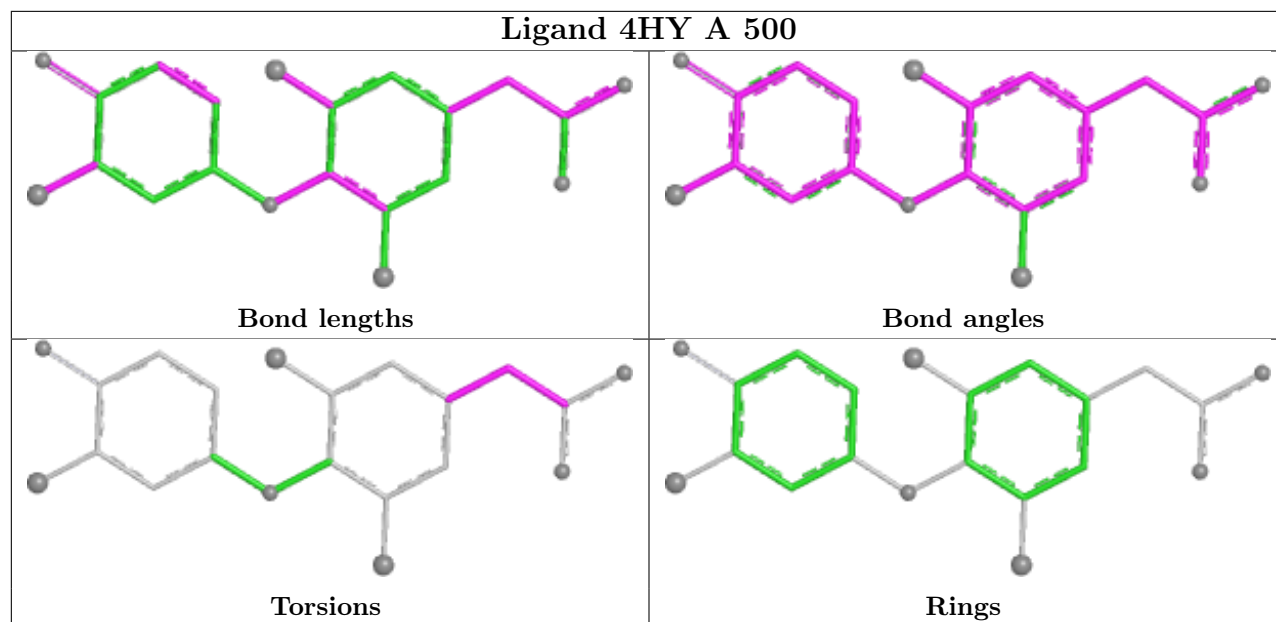
Mol	Chain	Res	Type	Atoms
2	A	500	4HY	C3-C1-C13-C14
2	A	500	4HY	C11-C1-C13-C14
2	A	500	4HY	C1-C13-C14-O3
2	A	500	4HY	C1-C13-C14-O4

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	4HY	8	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.