



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:52 AM GMT

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

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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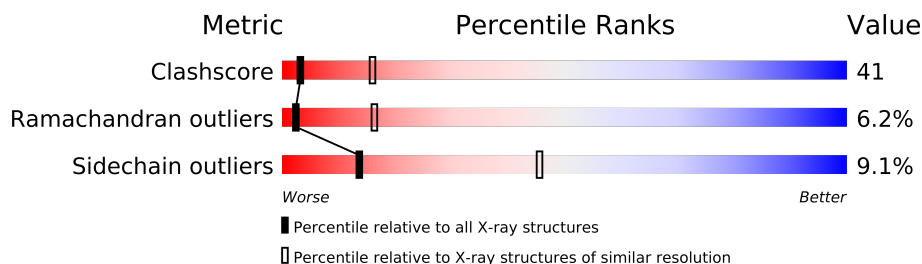
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

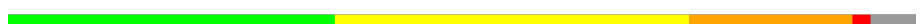
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 1908 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

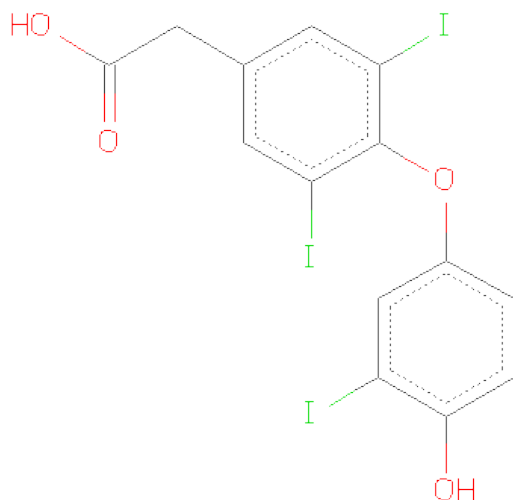
- Molecule 1 is a protein called Thyroid hormone receptor beta-1.

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 (three-letter code: 4HY) (formula: C<sub>14</sub>H<sub>9</sub>I<sub>3</sub>O<sub>4</sub>).



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

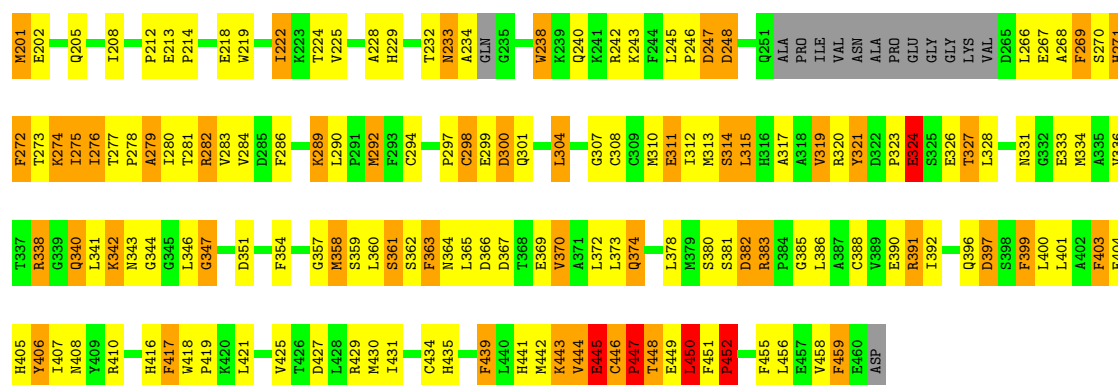
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

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 will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.27Å 67.27Å 130.12Å 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	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 <sup>2</sup> )	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	1.97	42/1930 (2.2%)	1.44	16/2621 (0.6%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	CYS	CB-SG	9.83	1.99	1.82
1	A	434	CYS	C-O	-8.41	1.07	1.23
1	A	321	TYR	CE2-CZ	-8.40	1.27	1.38
1	A	406	TYR	CE2-CZ	-8.12	1.27	1.38
1	A	445	GLU	CD-OE1	7.80	1.34	1.25
1	A	382	ASP	CB-CG	7.49	1.67	1.51
1	A	417	PHE	CE1-CZ	-7.42	1.23	1.37
1	A	319	VAL	CA-CB	-6.96	1.40	1.54
1	A	459	PHE	CE2-CZ	-6.81	1.24	1.37
1	A	282	ARG	CA-CB	6.67	1.68	1.53
1	A	383	ARG	CG-CD	-6.59	1.35	1.51
1	A	314	SER	C-O	6.59	1.35	1.23
1	A	289	LYS	C-O	6.46	1.35	1.23
1	A	418	TRP	CG-CD1	-6.41	1.27	1.36
1	A	370	VAL	CB-CG1	-6.23	1.39	1.52
1	A	222	ILE	C-O	-6.17	1.11	1.23
1	A	233	ASN	CA-C	6.06	1.68	1.52
1	A	439	PHE	CE1-CZ	-6.02	1.25	1.37
1	A	417	PHE	CG-CD2	-5.92	1.29	1.38
1	A	418	TRP	CE3-CZ3	-5.75	1.28	1.38
1	A	269	PHE	CG-CD2	-5.71	1.30	1.38
1	A	233	ASN	C-O	5.62	1.34	1.23
1	A	399	PHE	CE2-CZ	-5.55	1.26	1.37
1	A	321	TYR	CG-CD2	-5.52	1.31	1.39
1	A	406	TYR	CE1-CZ	-5.47	1.31	1.38
1	A	238	TRP	CZ3-CH2	-5.46	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ALA	CA-CB	-5.41	1.41	1.52
1	A	202	GLU	CD-OE2	-5.40	1.19	1.25
1	A	363	PHE	CD2-CE2	-5.37	1.28	1.39
1	A	447	PRO	CA-C	5.35	1.63	1.52
1	A	390	GLU	CG-CD	5.33	1.59	1.51
1	A	417	PHE	C-O	-5.27	1.13	1.23
1	A	272	PHE	CE2-CZ	5.24	1.47	1.37
1	A	340	GLN	C-O	-5.23	1.13	1.23
1	A	213	GLU	C-O	-5.21	1.13	1.23
1	A	364	ASN	C-O	-5.19	1.13	1.23
1	A	321	TYR	CG-CD1	-5.19	1.32	1.39
1	A	292	MET	CG-SD	5.17	1.94	1.81
1	A	347	GLY	C-O	-5.10	1.15	1.23
1	A	361	SER	CB-OG	5.08	1.48	1.42
1	A	374	GLN	CB-CG	5.03	1.66	1.52
1	A	406	TYR	CZ-OH	-5.02	1.29	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ASP	CB-CG-OD1	13.53	130.47	118.30
1	A	367	ASP	CB-CG-OD2	9.97	127.27	118.30
1	A	391	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	427	ASP	CB-CG-OD2	8.82	126.24	118.30
1	A	300	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	298	CYS	CA-CB-SG	7.48	127.46	114.00
1	A	311	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	A	447	PRO	N-CD-CG	-5.80	94.50	103.20
1	A	447	PRO	N-CA-C	5.77	127.09	112.10
1	A	338	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	391	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	450	LEU	CA-CB-CG	5.19	127.25	115.30
1	A	351	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	397	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	315	LEU	CB-CG-CD2	-5.02	102.46	111.00
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1887	0	1817	152	0
2	A	21	0	7	8	0
All	All	1908	0	1824	152	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (152) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:CG	1:A:201:MET:O	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:307:GLY:HA3	1:A:383:ARG:HD2	1.70	0.73
1:A:297:PRO:O	1:A:301:GLN:HG3	1.90	0.71
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:247:ASP:OD1	1:A:247:ASP:C	2.30	0.69
1:A:276:ILE:HD13	2:A:500:4HY:I1	2.62	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:LEU:O	1:A:362:SER:N	2.27	0.67
1:A:416:HIS:C	1:A:419:PRO:HD2	2.13	0.67
1:A:342:LYS:HG3	1:A:347:GLY:HA2	1.77	0.66
1:A:388:CYS:SG	1:A:391:ARG:NH1	2.70	0.65
1:A:416:HIS:O	1:A:417:PHE:C	2.35	0.65
1:A:276:ILE:HD11	2:A:500:4HY:C5	2.25	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:380:SER:HB2	1:A:383:ARG:HE	1.62	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
1:A:266:LEU:HD21	1:A:445:GLU:HG3	1.82	0.62
1:A:242:ARG:O	1:A:242:ARG:HG3	1.99	0.62
1:A:445:GLU:O	1:A:445:GLU:HG2	1.99	0.62
1:A:360:LEU:C	1:A:362:SER:H	2.04	0.61
1:A:272:PHE:HE1	1:A:344:GLY:HA3	1.65	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:HG2	1:A:429:ARG:HH11	1.67	0.59
1:A:238:TRP:C	1:A:240:GLN:N	2.54	0.59
1:A:341:LEU:HG	1:A:346:LEU:HD12	1.85	0.59
1:A:238:TRP:C	1:A:240:GLN:H	2.05	0.58
1:A:268:ALA:O	1:A:269:PHE:C	2.35	0.58
1:A:280:ILE:HG22	1:A:280:ILE:O	2.04	0.58
1:A:315:LEU:O	1:A:319:VAL:HG22	2.03	0.58
1:A:331:ASN:O	1:A:331:ASN:CG	2.42	0.58
1:A:404:GLU:O	1:A:407:ILE:HB	2.03	0.57
1:A:214:PRO:HB2	1:A:219:TRP:CE2	2.39	0.57
1:A:286:PHE:C	1:A:286:PHE:CD1	2.78	0.56
1:A:286:PHE:CE1	1:A:290:LEU:HD11	2.40	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:444:VAL:C	1:A:446:CYS:H	2.10	0.55
1:A:451:PHE:CD2	1:A:456:LEU:HD21	2.41	0.54
1:A:270:SER:O	1:A:273:THR:HB	2.07	0.54
1:A:218:GLU:O	1:A:222:ILE:HG13	2.08	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:416:HIS:O	1:A:419:PRO:CD	2.46	0.53
1:A:273:THR:CG2	1:A:452:PRO:CD	2.86	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:444:VAL:C	1:A:446:CYS:N	2.62	0.53
1:A:280:ILE:CG2	1:A:280:ILE:O	2.56	0.53
1:A:271:HIS:O	1:A:272:PHE:C	2.48	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:360:LEU:C	1:A:362:SER:N	2.63	0.51
1:A:233:ASN:O	1:A:234:ALA:C	2.48	0.51
1:A:300:ASP:O	1:A:301:GLN:C	2.46	0.51
1:A:240:GLN:HA	1:A:240:GLN:NE2	2.26	0.51
1:A:277:THR:N	1:A:278:PRO:CD	2.72	0.51
1:A:366:ASP:OD2	1:A:410:ARG:HD3	2.11	0.51
1:A:208:ILE:O	1:A:208:ILE:HG22	2.11	0.51
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:388:CYS:O	1:A:392:ILE:HG13	2.13	0.49
1:A:273:THR:HG23	1:A:452:PRO:CD	2.42	0.49
1:A:225:VAL:CG2	1:A:399:PHE:HE2	2.24	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:458:VAL:HG12	1:A:459:PHE:CD2	2.49	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:228:ALA:O	1:A:229:HIS:C	2.52	0.47
1:A:232:THR:HG23	1:A:289:LYS:HZ2	1.79	0.47
1:A:267:GLU:O	1:A:270:SER:CB	2.55	0.47
1:A:275:ILE:HG13	1:A:275:ILE:O	2.14	0.47
1:A:246:PRO:O	1:A:247:ASP:C	2.51	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:225:VAL:HG21	1:A:399:PHE:CE2	2.45	0.46
1:A:327:THR:HB	1:A:336:VAL:O	2.16	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:311:GLU:CD	1:A:383:ARG:HH22	2.20	0.46
1:A:331:ASN:O	1:A:333:GLU:HG3	2.16	0.46
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:310:MET:HG2	1:A:435:HIS:CB	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:430:MET:O	1:A:431:ILE:C	2.52	0.45
1:A:447:PRO:HB2	1:A:448:THR:H	1.36	0.45
1:A:406:TYR:CE2	1:A:410:ARG:HG3	2.52	0.45
1:A:274:LYS:C	1:A:276:ILE:H	2.21	0.44
1:A:443:LYS:O	1:A:447:PRO:HD3	2.17	0.44
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.50	0.44
1:A:366:ASP:OD1	1:A:369:GLU:HG3	2.16	0.44
1:A:319:VAL:HG23	1:A:320:ARG:N	2.33	0.44
1:A:341:LEU:CG	1:A:346:LEU:HD12	2.47	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:271:HIS:HB3	1:A:334:MET:CE	2.48	0.44
1:A:417:PHE:CE2	1:A:421:LEU:HD22	2.53	0.44
1:A:357:GLY:O	1:A:358:MET:C	2.54	0.43
1:A:385:GLY:O	1:A:386:LEU:C	2.56	0.43
1:A:365:LEU:HB3	1:A:369:GLU:HB2	1.99	0.43
1:A:286:PHE:O	1:A:286:PHE:CD1	2.71	0.43
1:A:429:ARG:HG2	1:A:429:ARG:NH1	2.32	0.43
1:A:396:GLN:O	1:A:397:ASP:C	2.57	0.43
1:A:271:HIS:O	1:A:274:LYS:N	2.52	0.43
1:A:357:GLY:O	1:A:359:SER:N	2.52	0.43
1:A:430:MET:HE3	1:A:430:MET:HA	2.01	0.42
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:363:PHE:CD1	1:A:421:LEU:HD13	2.54	0.42
1:A:321:TYR:HB2	1:A:328:LEU:HD23	2.01	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:346:LEU:O	1:A:347:GLY:C	2.59	0.41
1:A:232:THR:HG23	1:A:289:LYS:NZ	2.34	0.41
1:A:372:LEU:O	1:A:373:LEU:C	2.59	0.41
1:A:439:PHE:HA	1:A:442:MET:HE3	2.02	0.41
1:A:407:ILE:HA	1:A:407:ILE:HD13	1.79	0.41
1:A:369:GLU:O	1:A:370:VAL:C	2.57	0.41
1:A:442:MET:C	1:A:444:VAL:N	2.73	0.41
1:A:292:MET:SD	1:A:399:PHE:CE1	3.13	0.41
1:A:373:LEU:O	1:A:374:GLN:C	2.55	0.41
1:A:397:ASP:HA	1:A:400:LEU:HD12	2.02	0.41
1:A:324:GLU:C	1:A:326:GLU:H	2.23	0.41
1:A:246:PRO:O	1:A:248:ASP:N	2.53	0.40
1:A:338:ARG:HA	1:A:354:PHE:CE1	2.56	0.40
1:A:455:PHE:O	1:A:459:PHE:HD1	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:THR:O	1:A:282:ARG:C	2.59	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%)	2	16

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%)	179 (91%)	18 (9%)	14	45

All (18) 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	324	GLU
1	A	327	THR
1	A	358	MET
1	A	381	SER
1	A	382	ASP
1	A	403	PHE
1	A	445	GLU
1	A	450	LEU
1	A	452	PRO

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

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	2.94	6 (27%)	31,31,31	3.12	16 (51%)

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	-	-	0/8/8/8	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	4HY	O1-C8	-8.38	1.19	1.36
2	A	500	4HY	C13-C14	-6.98	1.33	1.50
2	A	500	4HY	O4-C14	-5.62	1.10	1.30
2	A	500	4HY	O2-C7	-2.79	1.34	1.39
2	A	500	4HY	C13-C1	2.69	1.56	1.51
2	A	500	4HY	C12-C10	2.28	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	4HY	C1-C13-C14	7.55	130.97	113.58
2	A	500	4HY	C13-C1-C3	7.04	131.28	120.43
2	A	500	4HY	O3-C14-C13	5.85	137.57	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	4HY	C10-C8-C6	-4.66	114.52	119.32
2	A	500	4HY	O4-C14-O3	-4.43	112.03	123.30
2	A	500	4HY	C12-C2-C4	-4.32	114.35	120.56
2	A	500	4HY	C13-C1-C11	-3.72	114.71	120.43
2	A	500	4HY	C12-C10-C8	3.67	124.49	120.50
2	A	500	4HY	C11-C1-C3	-3.29	114.00	118.95
2	A	500	4HY	O2-C7-C5	3.00	125.72	120.47
2	A	500	4HY	C2-C4-C6	2.61	126.89	118.97
2	A	500	4HY	O2-C7-C9	-2.37	116.32	120.47
2	A	500	4HY	C1-C3-C5	2.26	125.67	120.26
2	A	500	4HY	C1-C11-C9	2.16	125.42	120.26
2	A	500	4HY	C8-C6-I2	2.13	122.71	119.84
2	A	500	4HY	O1-C8-C6	2.12	122.62	119.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.