



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:18 PM GMT

PDB ID : 4Y4R  
Title : Crystal structure of ribosomal oxygenase NO66 dimer mutant  
Authors : Wang, C.; Hang, T.; Zang, J.  
Deposited on : 2015-02-11  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

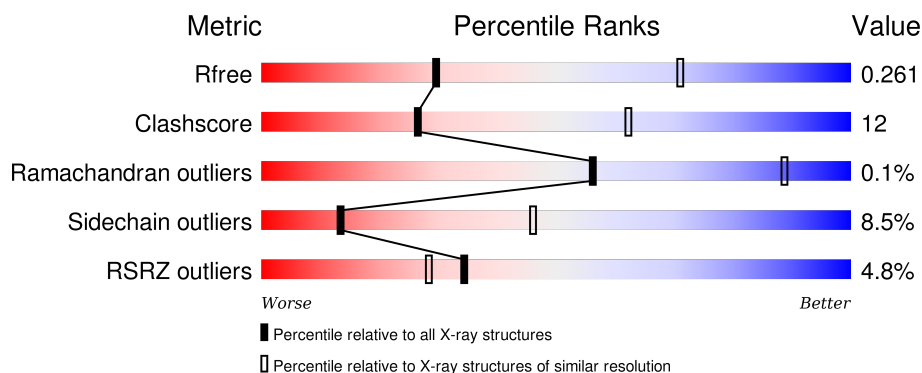
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. 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	454	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	454	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>6%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7082 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 Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3549	2255	625	654	15			
1	B	442	Total	C	N	O	S	0	0	0
			3523	2240	621	647	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	GLY	-	linker	UNP Q9H6W3
A	527	GLY	-	linker	UNP Q9H6W3
A	528	GLY	-	linker	UNP Q9H6W3
B	526	GLY	-	linker	UNP Q9H6W3
B	527	GLY	-	linker	UNP Q9H6W3
B	528	GLY	-	linker	UNP Q9H6W3

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

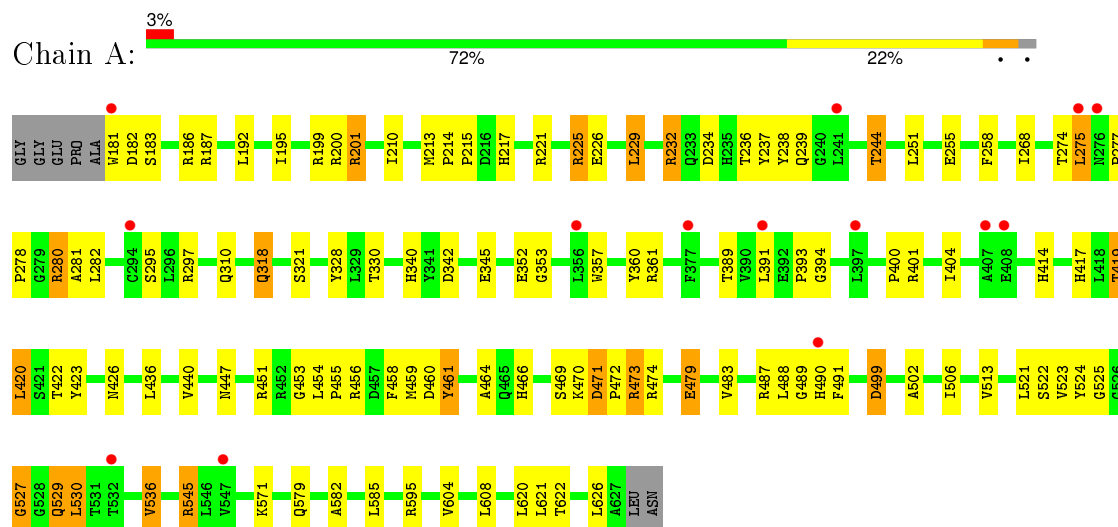
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	3	Total	O	0	0
			3	3		

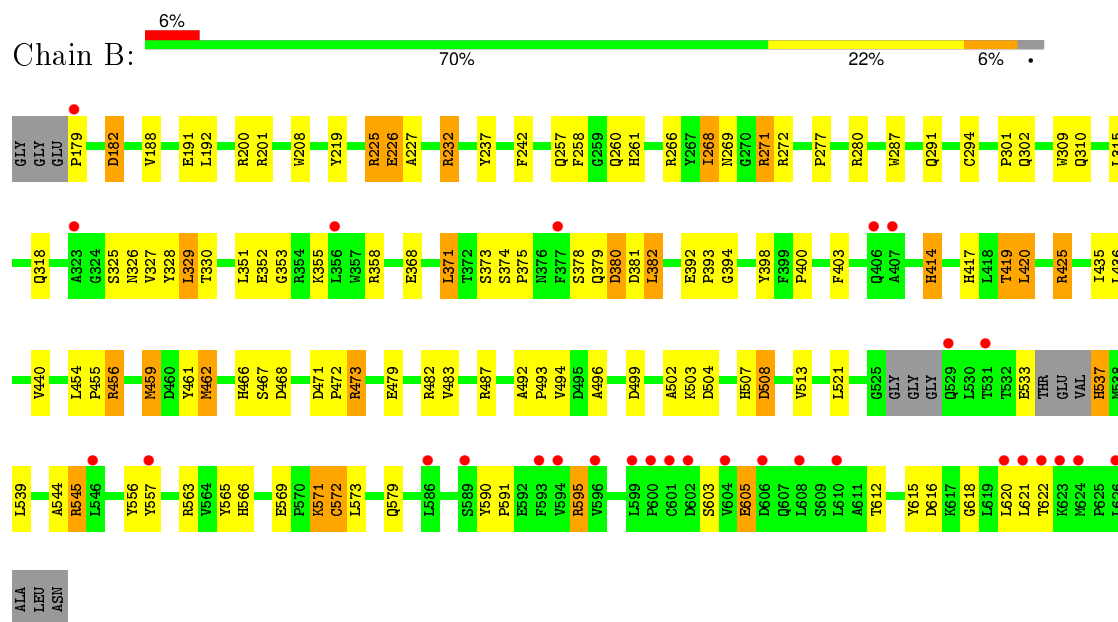
### 3 Residue-property plots

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.

- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66



- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.06 Å 144.21 Å 144.21 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 64.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.30) 98.5 (64.49-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.33 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.217 , 0.271 0.214 , 0.261	Depositor DCC
$R_{free}$ test set	1372 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.5	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27282 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, ACT

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	0.86	8/3640 (0.2%)	0.87	5/4954 (0.1%)
1	B	0.73	10/3615 (0.3%)	0.78	2/4918 (0.0%)
All	All	0.80	18/7255 (0.2%)	0.83	7/9872 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	GLU	CD-OE1	19.06	1.46	1.25
1	A	479	GLU	CD-OE2	14.85	1.42	1.25
1	A	479	GLU	CG-CD	13.50	1.72	1.51
1	B	605	GLU	CD-OE1	11.21	1.38	1.25
1	B	479	GLU	CD-OE1	10.30	1.36	1.25
1	B	605	GLU	CD-OE2	8.90	1.35	1.25
1	B	479	GLU	CD-OE2	8.50	1.35	1.25
1	B	579	GLN	CD-OE1	8.40	1.42	1.24
1	A	579	GLN	CD-OE1	8.12	1.41	1.24
1	B	179	PRO	N-CA	8.01	1.60	1.47
1	B	479	GLU	CG-CD	7.43	1.63	1.51
1	A	527	GLY	N-CA	7.32	1.57	1.46
1	B	605	GLU	CG-CD	7.13	1.62	1.51
1	A	579	GLN	CG-CD	5.88	1.64	1.51
1	B	579	GLN	CD-NE2	5.87	1.47	1.32
1	A	527	GLY	C-O	5.67	1.32	1.23
1	B	179	PRO	C-O	5.07	1.33	1.23
1	A	490	HIS	CA-CB	5.03	1.65	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ASP	CB-CG-OD1	6.38	124.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	HIS	CB-CA-C	5.75	121.91	110.40
1	A	525	GLY	N-CA-C	5.68	127.29	113.10
1	A	201	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	268	ILE	CB-CA-C	-5.18	101.25	111.60
1	A	420	LEU	CA-CB-CG	5.10	127.04	115.30
1	B	487	ARG	NE-CZ-NH1	-5.03	117.79	120.30

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	3549	0	3439	92	0
1	B	3523	0	3394	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	3	0	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
All	All	7082	0	6836	169	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 12.

All (169) 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:502:ALA:HA	1:B:459:MET:HE1	1.58	0.86
1:A:466:HIS:HB3	1:A:469:SER:OG	1.76	0.86
1:A:353:GLY:O	1:A:393:PRO:HD3	1.82	0.80
1:A:536:VAL:HG21	1:A:620:LEU:HD21	1.65	0.79
1:A:502:ALA:HA	1:B:459:MET:CE	2.11	0.79
1:B:269:ASN:O	1:B:271:ARG:NH1	2.16	0.79
1:A:295:SER:OG	1:A:330:THR:OG1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:TYR:O	1:A:474:ARG:NH1	2.25	0.69
1:A:458:PHE:HA	1:A:461:TYR:CE2	2.28	0.69
1:A:455:PRO:HG2	1:A:458:PHE:HB3	1.75	0.69
1:A:426:ASN:O	1:B:454:LEU:HD12	1.93	0.68
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.76	0.68
1:B:226:GLU:OE1	1:B:227:ALA:N	2.27	0.68
1:A:464:ALA:N	1:B:499:ASP:OD2	2.27	0.68
1:A:499:ASP:OD1	1:A:545:ARG:NH1	2.27	0.65
1:B:499:ASP:OD1	1:B:545:ARG:NH1	2.30	0.64
1:A:451:ARG:NH1	1:B:368:GLU:O	2.31	0.64
1:B:225:ARG:HH11	1:B:225:ARG:HG3	1.62	0.63
1:A:232:ARG:HD2	1:A:394:GLY:O	1.99	0.63
1:A:353:GLY:HA3	1:A:414:HIS:O	2.00	0.62
1:A:530:LEU:N	1:A:530:LEU:HD23	2.15	0.61
1:A:471:ASP:OD1	1:A:473:ARG:HD3	2.01	0.60
1:A:422:THR:OG1	1:A:423:TYR:N	2.35	0.60
1:B:260:GLN:OE1	1:B:261:HIS:NE2	2.35	0.60
1:A:181:TRP:O	1:A:186:ARG:HD3	2.02	0.60
1:B:425:ARG:HA	1:B:425:ARG:NE	2.17	0.59
1:A:213:MET:HG3	1:A:214:PRO:HD2	1.83	0.59
1:B:287:TRP:O	1:B:291:GLN:HG2	2.03	0.58
1:B:537:HIS:CE1	1:B:621:LEU:HD11	2.38	0.58
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.84	0.58
1:B:461:TYR:C	1:B:462:MET:HG2	2.24	0.58
1:B:309:TRP:CG	1:B:563:ARG:HD2	2.39	0.57
1:A:523:VAL:O	1:A:523:VAL:HG22	2.03	0.57
1:A:423:TYR:OH	1:B:456:ARG:HG3	2.05	0.57
1:A:479:GLU:O	1:A:483:VAL:HG12	2.05	0.56
1:A:582:ALA:O	1:A:585:LEU:HB3	2.06	0.56
1:A:545:ARG:CG	1:A:545:ARG:HH11	2.18	0.56
1:B:471:ASP:OD1	1:B:472:PRO:HD2	2.06	0.56
1:B:232:ARG:HD2	1:B:394:GLY:O	2.06	0.56
1:B:435:ILE:HD12	1:B:492:ALA:HB1	1.86	0.56
1:B:379:GLN:HA	1:B:382:LEU:CD1	2.36	0.55
1:B:353:GLY:O	1:B:393:PRO:HD3	2.07	0.55
1:A:621:LEU:HD12	1:A:621:LEU:C	2.28	0.54
1:B:456:ARG:HG2	1:B:456:ARG:HH11	1.73	0.54
1:A:275:LEU:HD12	1:A:275:LEU:H	1.73	0.54
1:A:229:LEU:HD13	1:A:389:THR:HG21	1.90	0.54
1:B:301:PRO:HG3	1:B:327:VAL:HG23	1.90	0.53
1:B:266:ARG:HB3	1:B:268:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:CD1	1:B:440:VAL:HG21	2.38	0.53
1:A:447:ASN:OD1	1:A:447:ASN:C	2.46	0.53
1:A:536:VAL:HG23	1:A:620:LEU:HG	1.91	0.53
1:B:325:SER:C	1:B:326:ASN:HD22	2.13	0.53
1:A:455:PRO:CG	1:A:458:PHE:HB3	2.38	0.52
1:B:208:TRP:CZ2	1:B:237:TYR:CE1	2.97	0.52
1:A:183:SER:CB	1:A:239:GLN:HB2	2.40	0.52
1:A:277:PRO:O	1:A:278:PRO:C	2.47	0.51
1:B:621:LEU:HD12	1:B:621:LEU:O	2.10	0.51
1:A:234:ASP:OD2	1:A:236:THR:OG1	2.18	0.51
1:A:297:ARG:HG3	1:A:328:TYR:CE1	2.46	0.51
1:A:530:LEU:HD22	1:A:626:LEU:HD11	1.91	0.51
1:A:244:THR:OG1	1:A:352:GLU:OE1	2.26	0.51
1:B:232:ARG:HD3	1:B:237:TYR:CG	2.46	0.51
1:B:182:ASP:OD1	1:B:182:ASP:N	2.43	0.51
1:B:493:PRO:HB2	1:B:496:ALA:HB3	1.94	0.50
1:B:456:ARG:CG	1:B:456:ARG:HH11	2.23	0.50
1:A:251:LEU:O	1:A:280:ARG:NH1	2.45	0.49
1:A:464:ALA:H	1:B:499:ASP:CG	2.13	0.49
1:B:371:LEU:H	1:B:371:LEU:HD12	1.77	0.49
1:B:329:LEU:HD12	1:B:330:THR:N	2.27	0.49
1:A:502:ALA:HA	1:B:459:MET:HE2	1.90	0.49
1:B:266:ARG:HD2	1:B:268:ILE:HD11	1.94	0.49
1:A:210:ILE:HD11	1:A:215:PRO:HA	1.95	0.49
1:B:508:ASP:OD1	1:B:565:TYR:HE1	1.95	0.49
1:A:275:LEU:HD12	1:A:275:LEU:N	2.27	0.49
1:A:345:GLU:OE2	1:A:401:ARG:NH1	2.44	0.49
1:A:182:ASP:OD2	1:A:187:ARG:NH1	2.46	0.49
1:A:436:LEU:HD12	1:B:440:VAL:HG21	1.95	0.48
1:A:357:TRP:CD1	1:A:391:LEU:HD12	2.48	0.48
1:B:504:ASP:O	1:B:508:ASP:HB2	2.13	0.48
1:B:503:LYS:HD2	1:B:556:TYR:CE1	2.48	0.48
1:B:398:TYR:CD2	1:B:398:TYR:C	2.87	0.48
1:A:440:VAL:HA	1:A:488:LEU:HD21	1.95	0.48
1:B:615:TYR:HA	1:B:620:LEU:HB3	1.95	0.48
1:A:488:LEU:HD11	1:B:436:LEU:HD11	1.95	0.47
1:B:260:GLN:OE1	1:B:261:HIS:CE1	2.68	0.47
1:A:502:ALA:CA	1:B:459:MET:CE	2.88	0.47
1:A:456:ARG:CZ	1:B:219:TYR:CE2	2.97	0.47
1:B:266:ARG:HB3	1:B:268:ILE:HD11	1.96	0.47
1:B:380:ASP:N	1:B:380:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ALA:CA	1:B:459:MET:HE2	2.45	0.47
1:B:309:TRP:CD2	1:B:563:ARG:HD2	2.50	0.47
1:A:226:GLU:OE1	1:A:361:ARG:NH2	2.49	0.46
1:A:340:HIS:O	1:A:404:ILE:HA	2.15	0.46
1:A:466:HIS:CB	1:A:469:SER:OG	2.56	0.46
1:A:436:LEU:CD1	1:B:440:VAL:CG2	2.93	0.46
1:A:417:HIS:CD2	1:A:419:THR:HG22	2.51	0.46
1:B:461:TYR:O	1:B:462:MET:HG2	2.15	0.46
1:A:360:TYR:HB2	1:A:404:ILE:HB	1.97	0.46
1:B:435:ILE:HD11	1:B:494:VAL:HA	1.98	0.45
1:B:454:LEU:O	1:B:455:PRO:C	2.54	0.45
1:B:392:GLU:O	1:B:393:PRO:C	2.55	0.45
1:B:539:LEU:HD22	1:B:618:GLY:O	2.17	0.45
1:A:502:ALA:O	1:A:506:ILE:HG12	2.16	0.45
1:A:426:ASN:C	1:B:454:LEU:HD12	2.37	0.45
1:B:507:HIS:CE1	1:B:566:HIS:CE1	3.05	0.45
1:B:352:GLU:OE1	1:B:414:HIS:HE1	1.99	0.45
1:B:533:GLU:OE2	1:B:595:ARG:NH1	2.50	0.45
1:A:345:GLU:OE1	1:A:400:PRO:HA	2.16	0.44
1:B:225:ARG:NH1	1:B:225:ARG:HG3	2.30	0.44
1:B:268:ILE:N	1:B:268:ILE:HD12	2.33	0.44
1:A:436:LEU:O	1:A:440:VAL:HG23	2.17	0.44
1:A:258:PHE:CE2	1:A:281:ALA:HB2	2.52	0.44
1:A:217:HIS:CE1	1:A:221:ARG:HD2	2.53	0.44
1:B:603:SER:CB	1:B:605:GLU:OE1	2.66	0.44
1:A:489:GLY:C	1:A:491:PHE:H	2.21	0.43
1:A:582:ALA:O	1:A:585:LEU:N	2.51	0.43
1:B:257:GLN:H	1:B:261:HIS:HD2	1.66	0.43
1:B:417:HIS:CD2	1:B:419:THR:HG22	2.54	0.43
1:B:471:ASP:CG	1:B:473:ARG:HE	2.20	0.43
1:A:453:GLY:C	1:A:454:LEU:O	2.56	0.43
1:B:257:GLN:H	1:B:261:HIS:CD2	2.37	0.43
1:A:318:GLN:O	1:B:456:ARG:NH1	2.52	0.43
1:A:527:GLY:O	1:A:626:LEU:HD13	2.19	0.42
1:B:266:ARG:HG3	1:B:294:CYS:SG	2.59	0.42
1:A:489:GLY:O	1:A:491:PHE:N	2.52	0.42
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.84	0.42
1:B:425:ARG:CA	1:B:425:ARG:NE	2.80	0.42
1:A:460:ASP:O	1:A:466:HIS:ND1	2.52	0.42
1:A:470:LYS:O	1:A:471:ASP:C	2.58	0.42
1:A:229:LEU:CD1	1:A:389:THR:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:THR:O	1:B:616:ASP:OD2	2.37	0.42
1:A:466:HIS:CD2	1:A:466:HIS:N	2.86	0.42
1:B:266:ARG:O	1:B:272:ARG:HA	2.20	0.42
1:A:521:LEU:HB3	1:A:622:THR:O	2.20	0.42
1:B:309:TRP:CE3	1:B:563:ARG:NH1	2.88	0.42
1:A:460:ASP:O	1:A:466:HIS:CE1	2.72	0.42
1:A:489:GLY:C	1:B:482:ARG:HD3	2.41	0.42
1:A:225:ARG:CG	1:A:225:ARG:HH11	2.32	0.42
1:B:569:GLU:O	1:B:571:LYS:HD2	2.20	0.42
1:B:315:LEU:HD13	1:B:420:LEU:HD11	2.01	0.42
1:B:378:SER:O	1:B:381:ASP:HB2	2.20	0.42
1:A:181:TRP:O	1:A:186:ARG:CD	2.68	0.41
1:B:466:HIS:C	1:B:468:ASP:H	2.23	0.41
1:A:522:SER:OG	1:A:524:TYR:HD2	2.03	0.41
1:B:557:TYR:CE1	1:B:571:LYS:HB3	2.55	0.41
1:B:572:CYS:SG	1:B:573:LEU:N	2.93	0.41
1:B:502:ALA:O	1:B:503:LYS:C	2.58	0.41
1:B:192:LEU:O	1:B:201:ARG:HD3	2.19	0.41
1:B:544:ALA:HA	1:B:556:TYR:O	2.20	0.41
1:A:213:MET:HG3	1:A:214:PRO:CD	2.49	0.41
1:A:536:VAL:HG21	1:A:620:LEU:CD2	2.43	0.41
1:B:379:GLN:HA	1:B:382:LEU:HD11	2.02	0.41
1:B:595:ARG:HE	1:B:595:ARG:HB3	1.56	0.41
1:A:237:TYR:HD1	1:A:238:TYR:CE1	2.39	0.41
1:B:188:VAL:O	1:B:191:GLU:HB3	2.21	0.41
1:A:502:ALA:HB2	1:B:459:MET:HE2	2.03	0.41
1:A:529:GLN:N	1:A:529:GLN:OE1	2.53	0.41
1:B:537:HIS:HD2	1:B:591:PRO:C	2.24	0.40
1:B:400:PRO:HD2	1:B:403:PHE:CE2	2.56	0.40
1:B:258:PHE:CE2	1:B:277:PRO:HG2	2.56	0.40
1:B:374:SER:HB2	1:B:375:PRO:HD2	2.03	0.40
1:A:461:TYR:HD1	1:A:474:ARG:HA	1.85	0.40
1:B:271:ARG:HD3	1:B:271:ARG:N	2.36	0.40
1:B:242:PHE:O	1:B:351:LEU:HD13	2.21	0.40
1:B:521:LEU:HB3	1:B:622:THR:O	2.22	0.40
1:A:195:ILE:HB	1:A:201:ARG:HG2	2.02	0.40
1:A:192:LEU:O	1:A:201:ARG:HD3	2.21	0.40
1:A:489:GLY:C	1:A:491:PHE:N	2.75	0.40
1:A:604:VAL:HG12	1:A:604:VAL:O	2.22	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	445/454 (98%)	407 (92%)	37 (8%)	1 (0%)	52	85
1	B	436/454 (96%)	389 (89%)	47 (11%)	0	100	100
All	All	881/908 (97%)	796 (90%)	84 (10%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	PRO

### 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	373/386 (97%)	344 (92%)	29 (8%)	16	50
1	B	369/386 (96%)	335 (91%)	34 (9%)	11	40
All	All	742/772 (96%)	679 (92%)	63 (8%)	13	46

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	A	200	ARG
1	A	225	ARG
1	A	229	LEU
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	244	THR
1	A	255	GLU
1	A	268	ILE
1	A	274	THR
1	A	275	LEU
1	A	280	ARG
1	A	282	LEU
1	A	318	GLN
1	A	321	SER
1	A	342	ASP
1	A	419	THR
1	A	420	LEU
1	A	459	MET
1	A	461	TYR
1	A	471	ASP
1	A	473	ARG
1	A	487	ARG
1	A	529	GLN
1	A	530	LEU
1	A	536	VAL
1	A	545	ARG
1	A	571	LYS
1	A	595	ARG
1	A	608	LEU
1	B	182	ASP
1	B	200	ARG
1	B	225	ARG
1	B	226	GLU
1	B	232	ARG
1	B	271	ARG
1	B	280	ARG
1	B	302	GLN
1	B	318	GLN
1	B	328	TYR
1	B	329	LEU
1	B	355	LYS
1	B	358	ARG
1	B	371	LEU
1	B	373	SER
1	B	380	ASP
1	B	382	LEU
1	B	414	HIS

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Mol	Chain	Res	Type
1	B	419	THR
1	B	420	LEU
1	B	425	ARG
1	B	456	ARG
1	B	459	MET
1	B	462	MET
1	B	467	SER
1	B	473	ARG
1	B	483	VAL
1	B	508	ASP
1	B	537	HIS
1	B	545	ARG
1	B	571	LYS
1	B	572	CYS
1	B	590	TYR
1	B	595	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	235	HIS
1	A	291	GLN
1	A	340	HIS
1	A	410	GLN
1	B	326	ASN
1	B	340	HIS
1	B	410	GLN
1	B	414	HIS
1	B	465	GLN
1	B	466	HIS
1	B	490	HIS
1	B	507	HIS
1	B	537	HIS
1	B	566	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	ACT	A	702	2	0,3,3	0.00	-	0,3,3	0.00	-

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	ACT	A	702	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	447/454 (98%)	0.42	14 (3%)	52 46	50, 87, 126, 167	1 (0%)
1	B	442/454 (97%)	0.53	29 (6%)	22 17	52, 111, 151, 173	0
All	All	889/908 (97%)	0.48	43 (4%)	34 28	50, 99, 146, 173	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	610	LEU	5.3
1	B	599	LEU	4.4
1	B	621	LEU	4.1
1	B	622	THR	3.9
1	B	608	LEU	3.3
1	B	594	VAL	3.1
1	B	602	ASP	3.0
1	B	600	PRO	2.9
1	B	606	ASP	2.9
1	B	406	GLN	2.9
1	B	601	CYS	2.9
1	A	356	LEU	2.8
1	B	604	VAL	2.8
1	A	275	LEU	2.7
1	B	546	LEU	2.7
1	A	276	ASN	2.6
1	B	377	PHE	2.6
1	B	179	PRO	2.6
1	A	391	LEU	2.6
1	B	626	LEU	2.6
1	A	377	PHE	2.5
1	B	623	LYS	2.5
1	B	407	ALA	2.5
1	B	596	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	620	LEU	2.4
1	A	407	ALA	2.4
1	A	408	GLU	2.4
1	A	181	TRP	2.3
1	B	356	LEU	2.3
1	B	529	GLN	2.2
1	A	532	THR	2.2
1	A	397	LEU	2.2
1	A	241	LEU	2.2
1	B	593	PHE	2.1
1	B	624	MET	2.1
1	A	547	VAL	2.1
1	B	589	SER	2.1
1	B	586	LEU	2.1
1	B	531	THR	2.1
1	B	557	TYR	2.0
1	A	490	HIS	2.0
1	B	323	ALA	2.0
1	A	294	CYS	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	A	702	4/4	0.96	0.20	-1.28	49,52,54,54	0
2	NI	B	701	1/1	0.99	0.20	-	102,102,102,102	0
2	NI	A	701	1/1	0.98	0.20	-	87,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.