



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:09 PM UTC

PDB ID : 4Y4R / pdb_00004y4r
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

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
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

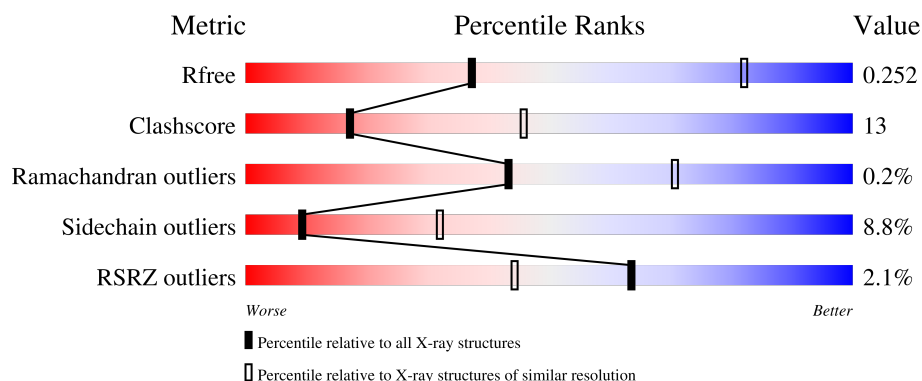
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	454	2% 70% 23% 5%
1	B	454	2% 68% 26% .

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 (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

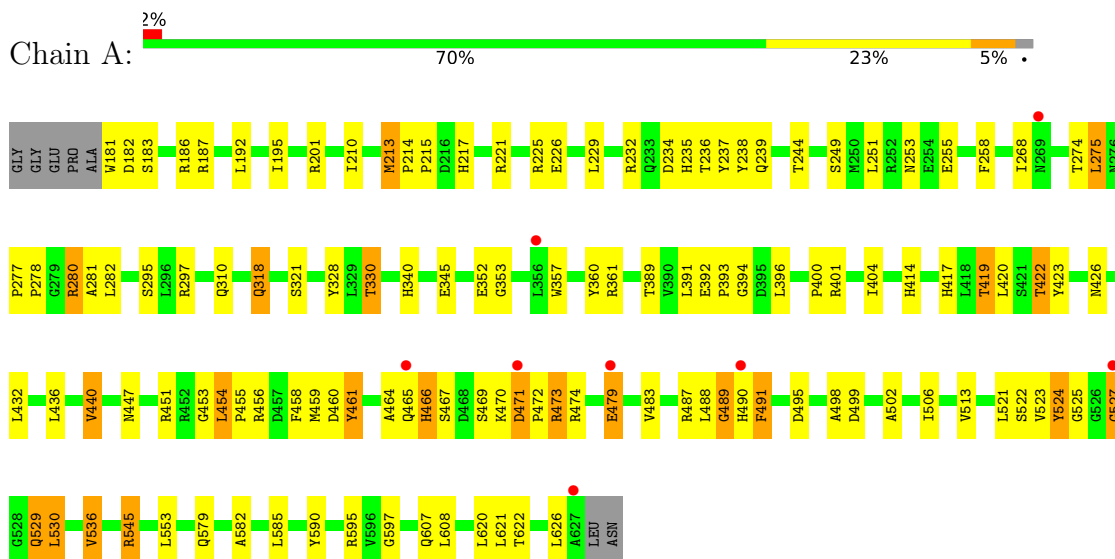
- Molecule 4 is water.

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

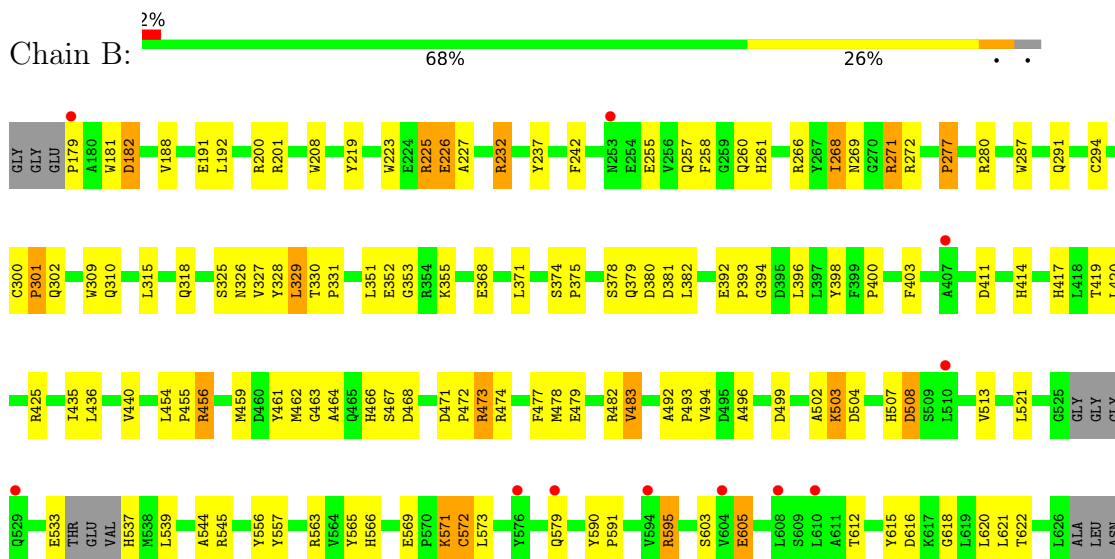
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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, α , β , γ	86.06Å 144.21Å 144.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.30) 98.4 (50.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.217 , 0.271 (Not available) , 0.252	Depositor DCC
R_{free} test set	1372 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	89.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7082	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.02	13/3640 (0.4%)	1.08	15/4954 (0.3%)
1	B	0.85	8/3615 (0.2%)	1.04	10/4918 (0.2%)
All	All	0.94	21/7255 (0.3%)	1.06	25/9872 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	GLY	N-CA	11.95	1.57	1.44
1	A	479	GLU	CD-OE1	11.19	1.46	1.25
1	B	579	GLN	CD-OE1	9.94	1.42	1.23
1	A	579	GLN	CD-OE1	9.61	1.41	1.23
1	B	179	PRO	N-CA	9.21	1.60	1.47
1	A	479	GLU	CD-OE2	8.75	1.42	1.25
1	A	490	HIS	CA-C	8.73	1.64	1.52
1	A	479	GLU	CG-CD	8.06	1.72	1.52
1	A	490	HIS	CA-CB	6.84	1.65	1.53
1	B	579	GLN	CD-NE2	6.80	1.47	1.33
1	B	605	GLU	CD-OE1	6.65	1.38	1.25
1	B	479	GLU	CD-OE1	6.12	1.36	1.25
1	A	491	PHE	N-CA	5.99	1.53	1.46
1	A	490	HIS	CB-CG	5.82	1.58	1.50
1	A	527	GLY	C-O	5.71	1.32	1.24
1	A	524	TYR	CA-C	5.66	1.60	1.52
1	A	527	GLY	CA-C	5.35	1.58	1.52
1	B	605	GLU	CD-OE2	5.31	1.35	1.25
1	B	301	PRO	N-CA	-5.16	1.44	1.47
1	B	479	GLU	CD-OE2	5.08	1.35	1.25
1	A	579	GLN	CG-CD	5.01	1.64	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	PRO	CA-C-N	-8.14	111.97	120.03
1	B	277	PRO	C-N-CA	-8.14	111.97	120.03
1	B	331	PRO	CA-C-N	6.80	128.34	119.84
1	B	331	PRO	C-N-CA	6.80	128.34	119.84
1	A	454	LEU	CA-C-N	-6.32	114.03	120.85
1	A	454	LEU	C-N-CA	-6.32	114.03	120.85
1	B	483	VAL	N-CA-CB	6.29	117.91	110.55
1	A	422	THR	N-CA-C	6.28	116.37	108.45
1	B	181	TRP	N-CA-C	6.02	117.73	109.18
1	A	525	GLY	N-CA-C	5.96	127.29	113.18
1	B	411	ASP	CB-CA-C	-5.86	109.80	116.54
1	A	467	SER	N-CA-C	-5.86	104.25	111.40
1	A	253	ASN	N-CA-C	5.83	120.09	112.92
1	A	235	HIS	N-CA-C	-5.79	105.32	112.90
1	A	490	HIS	CB-CA-C	5.77	121.91	110.42
1	B	300	CYS	N-CA-C	5.77	122.56	109.81
1	A	489	GLY	N-CA-C	-5.70	105.89	112.50
1	B	268	ILE	CB-CA-C	-5.52	101.25	111.18
1	B	477	PHE	N-CA-C	-5.49	105.19	111.07
1	A	440	VAL	CB-CA-C	-5.31	104.89	112.22
1	A	491	PHE	N-CA-C	5.15	120.21	112.94
1	A	213	MET	CA-C-N	-5.07	115.15	120.38
1	A	213	MET	C-N-CA	-5.07	115.15	120.38
1	A	498	ALA	N-CA-C	-5.06	105.03	111.11
1	A	590	TYR	N-CA-C	-5.06	103.41	109.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	101	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	3	0	0	0	0
All	All	7082	0	6836	175	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 13.

All (175) 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	1.51	0.93
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
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:B:462:MET:HE3	1:B:474:ARG:NH1	2.09	0.68
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.76	0.68
1:A:464:ALA:N	1:B:499:ASP:OD2	2.27	0.68
1:B:226:GLU:OE1	1:B:227:ALA:N	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:B:461:TYR:C	1:B:462:MET:HG2	2.24	0.62
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: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:NE	1:B:425:ARG:HA	2.17	0.59
1:A:621:LEU:C	1:A:621:LEU:HD12	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:THR:OG1	1:A:423:TYR:N	2.35	0.58
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.84	0.58
1:A:447:ASN:C	1:A:447:ASN:OD1	2.46	0.58
1:A:523:VAL:HG22	1:A:523:VAL:O	2.03	0.57
1:B:309:TRP:CG	1:B:563:ARG:HD2	2.39	0.57
1:B:325:SER:C	1:B:326:ASN:HD22	2.13	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:277:PRO:O	1:A:278:PRO:C	2.47	0.56
1:A:545:ARG:HH11	1:A:545:ARG:CG	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:464:ALA:H	1:B:499:ASP:CG	2.13	0.54
1:A:275:LEU:HD12	1:A:275:LEU:H	1.73	0.54
1:B:456:ARG:HH11	1:B:456:ARG:HG2	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
1:A:436:LEU:CD1	1:B:440:VAL:HG21	2.38	0.53
1:A:536:VAL:HG23	1:A:620:LEU:HG	1.91	0.53
1:B:398:TYR:CD2	1:B:398:TYR:C	2.87	0.52
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: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:B:621:LEU:HD12	1:B:621:LEU:O	2.10	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:N	1:B:182:ASP:OD1	2.43	0.51
1:B:493:PRO:HB2	1:B:496:ALA:HB3	1.94	0.50
1:B:456:ARG:HH11	1:B:456:ARG:CG	2.23	0.50
1:B:454:LEU:O	1:B:455:PRO:C	2.54	0.50
1:B:392:GLU:O	1:B:393:PRO:C	2.55	0.50
1:A:426:ASN:C	1:B:454:LEU:HD12	2.37	0.50
1:A:251:LEU:O	1:A:280:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:HD12	1:B:371:LEU:H	1.77	0.49
1:B:329:LEU:HD12	1:B:330:THR:N	2.27	0.49
1:A:210:ILE:HD11	1:A:215:PRO:HA	1.95	0.49
1:B:266:ARG:HD2	1:B:268:ILE:HD11	1.94	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:182:ASP:OD2	1:A:187:ARG:NH1	2.46	0.49
1:A:345:GLU:OE2	1:A:401:ARG:NH1	2.44	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:471:ASP:CG	1:B:473:ARG:HE	2.20	0.48
1:B:503:LYS:HD2	1:B:556:TYR:CE1	2.48	0.48
1:A:489:GLY:C	1:A:491:PHE:H	2.21	0.48
1:A:440:VAL:HA	1:A:488:LEU:HD21	1.95	0.48
1:A:453:GLY:C	1:A:454:LEU:O	2.56	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:456:ARG:CZ	1:B:219:TYR:CE2	2.97	0.47
1:A:502:ALA:CA	1:B:459:MET:CE	2.88	0.47
1:B:266:ARG:HB3	1:B:268:ILE:HD11	1.96	0.47
1:B:380:ASP:OD1	1:B:380:ASP:N	2.46	0.47
1:B:309:TRP:CD2	1:B:563:ARG:HD2	2.50	0.47
1:A:470:LYS:O	1:A:471:ASP:C	2.58	0.47
1:A:489:GLY:C	1:B:482:ARG:HD3	2.41	0.46
1:A:226:GLU:OE1	1:A:361:ARG:NH2	2.49	0.46
1:B:466:HIS:C	1:B:468:ASP:H	2.23	0.46
1:A:340:HIS:O	1:A:404:ILE:HA	2.15	0.46
1:A:417:HIS:CD2	1:A:419:THR:HG22	2.51	0.46
1:A:436:LEU:CD1	1:B:440:VAL:CG2	2.93	0.46
1:A:466:HIS:CB	1:A:469:SER:OG	2.56	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:502:ALA:O	1:B:503:LYS:C	2.58	0.45
1:B:537:HIS:HD2	1:B:591:PRO:C	2.24	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:B:352:GLU:OE1	1:B:414:HIS:HE1	1.99	0.45
1:B:507:HIS:CE1	1:B:566:HIS:CE1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLY:C	1:A:491:PHE:N	2.75	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:A:258:PHE:CE2	1:A:281:ALA:HB2	2.52	0.44
1:A:436:LEU:O	1:A:440:VAL:HG23	2.17	0.44
1:B:225:ARG:HG3	1:B:225:ARG:NH1	2.30	0.44
1:B:268:ILE:N	1:B:268:ILE:HD12	2.33	0.44
1:B:466:HIS:C	1:B:468:ASP:N	2.75	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:495:ASP:CG	1:B:474:ARG:HH22	2.26	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:257:GLN:H	1:B:261:HIS:CD2	2.37	0.43
1:A:597:GLY:C	1:A:607:GLN:NE2	2.77	0.43
1:B:573:LEU:C	1:B:573:LEU:HD12	2.44	0.43
1:A:318:GLN:O	1:B:456:ARG:NH1	2.52	0.43
1:A:225:ARG:HH11	1:A:225:ARG:HG3	1.84	0.42
1:A:489:GLY:O	1:A:491:PHE:N	2.52	0.42
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:B:425:ARG:NE	1:B:425:ARG:CA	2.80	0.42
1:A:460:ASP:O	1:A:466:HIS:ND1	2.52	0.42
1:B:309:TRP:CD1	1:B:309:TRP:C	2.97	0.42
1:A:229:LEU:CD1	1:A:389:THR:HG21	2.49	0.42
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:A:521:LEU:HB3	1:A:622:THR:O	2.20	0.42
1:B:266:ARG:O	1:B:272:ARG:HA	2.20	0.42
1:B:309:TRP:CE3	1:B:563:ARG:NH1	2.88	0.42
1:A:225:ARG:HH11	1:A:225:ARG:CG	2.32	0.42
1:A:460:ASP:O	1:A:466:HIS:CE1	2.72	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:B:569:GLU:O	1:B:571:LYS:HD2	2.20	0.42
1:A:181:TRP:O	1:A:186:ARG:CD	2.68	0.41
1:B:463:GLY:O	1:B:464:ALA:C	2.63	0.41
1:A:522:SER:OG	1:A:524:TYR:HD2	2.03	0.41
1:A:392:GLU:O	1:A:393:PRO:C	2.61	0.41
1:B:557:TYR:CE1	1:B:571:LYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:CYS:SG	1:B:573:LEU:N	2.93	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:237:TYR:HD1	1:A:238:TYR:CE1	2.39	0.41
1:A:536:VAL:HG21	1:A:620:LEU:CD2	2.43	0.41
1:B:188:VAL:O	1:B:191:GLU:HB3	2.21	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:529:GLN:OE1	1:A:529:GLN:N	2.53	0.41
1:B:223:TRP:C	1:B:225:ARG:H	2.29	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:B:400:PRO:HD2	1:B:403:PHE:CE2	2.56	0.40
1:A:461:TYR:HD1	1:A:474:ARG:HA	1.85	0.40
1:A:502:ALA:HA	1:B:459:MET:HE2	1.98	0.40
1:B:242:PHE:O	1:B:351:LEU:HD13	2.21	0.40
1:B:271:ARG:N	1:B:271:ARG:HD3	2.36	0.40
1:A:192:LEU:O	1:A:201:ARG:HD3	2.21	0.40
1:A:195:ILE:HB	1:A:201:ARG:HG2	2.02	0.40
1:B:521:LEU:HB3	1:B:622:THR: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%)	43	71
1	B	184/454 (40%)	163 (89%)	21 (11%)	0	100	100
All	All	629/908 (69%)	570 (91%)	58 (9%)	1 (0%)	43	71

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	320/386 (83%)	292 (91%)	28 (9%)	9	32
1	B	284/386 (74%)	259 (91%)	25 (9%)	9	32
All	All	604/772 (78%)	551 (91%)	53 (9%)	9	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	SER
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	330	THR
1	A	396	LEU
1	A	419	THR
1	A	420	LEU
1	A	432	LEU
1	A	459	MET
1	A	461	TYR
1	A	465	GLN
1	A	466	HIS
1	A	471	ASP
1	A	473	ARG
1	A	487	ARG
1	A	529	GLN

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Mol	Chain	Res	Type
1	A	530	LEU
1	A	536	VAL
1	A	545	ARG
1	A	553	LEU
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	255	GLU
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	396	LEU
1	B	456	ARG
1	B	467	SER
1	B	473	ARG
1	B	478	MET
1	B	483	VAL
1	B	503	LYS
1	B	508	ASP
1	B	571	LYS
1	B	572	CYS
1	B	590	TYR
1	B	595	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	A	318	GLN
1	A	340	HIS
1	A	410	GLN
1	A	579	GLN
1	B	235	HIS
1	B	318	GLN

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Mol	Chain	Res	Type
1	B	326	ASN
1	B	340	HIS
1	B	490	HIS
1	B	507	HIS
1	B	566	HIS
1	B	579	GLN

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 [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	3,3,3	1.50	1 (33%)	3,3,3	0.39	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ACT	O-C	2.27	1.32	1.22

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	447/454 (98%)	-0.07	8 (1%) 67 49	50, 87, 126, 167	1 (0%)
1	B	442/454 (97%)	0.17	11 (2%) 58 39	52, 111, 151, 173	0
All	All	889/908 (97%)	0.05	19 (2%) 63 44	50, 99, 146, 173	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	PRO	3.7
1	A	490	HIS	3.5
1	B	608	LEU	3.0
1	A	479	GLU	2.8
1	A	269	ASN	2.6
1	A	471	ASP	2.5
1	A	627	ALA	2.4
1	B	610	LEU	2.3
1	B	579	GLN	2.3
1	A	465	GLN	2.3
1	B	407	ALA	2.2
1	A	527	GLY	2.2
1	A	356	LEU	2.2
1	B	253	ASN	2.2
1	B	594	VAL	2.1
1	B	604	VAL	2.1
1	B	576	TYR	2.1
1	B	529	GLN	2.1
1	B	510	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
3	ACT	A	702	4/4	0.88	0.13	49,52,54,54	0
2	NI	B	701	1/1	0.99	0.03	102,102,102,102	0
2	NI	A	701	1/1	0.99	0.05	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.