



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 4DIQ / pdb_00004diq
Title : Crystal Structure of human NO66
Authors : Vollmar, M.; Krojer, T.; Ng, S.; Pilka, E.; Bray, J.; Pike, A.C.W.; Filipakopoulos, P.; Roos, A.; Arrowsmith, C.H.; Edwards, E.; Bountra, C.; von Delft, F.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2012-01-31
Resolution : 2.40 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

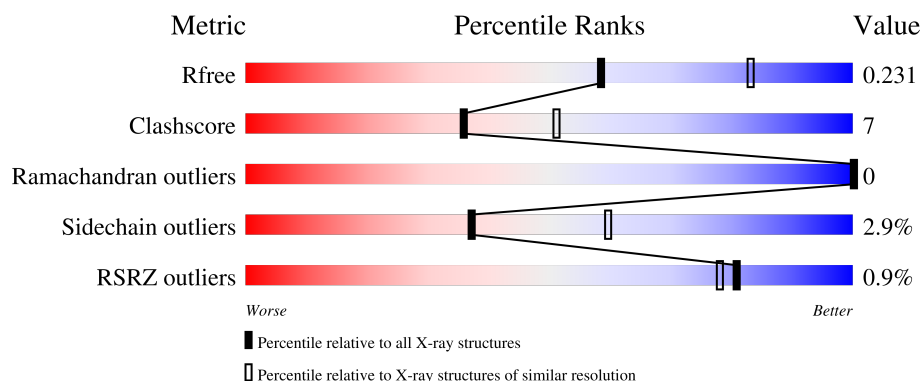
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

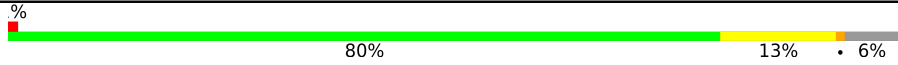
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	489	
1	B	489	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7412 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 Lysine-specific demethylase NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	2	0
			3618	2310	634	660	14			
1	B	457	Total	C	N	O	S	0	3	0
			3643	2324	639	664	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	LEU	-	expression tag	UNP Q9H6W3
A	161	ARG	-	expression tag	UNP Q9H6W3
A	162	ARG	-	expression tag	UNP Q9H6W3
A	163	ARG	-	expression tag	UNP Q9H6W3
A	164	TYR	-	expression tag	UNP Q9H6W3
A	165	THR	-	expression tag	UNP Q9H6W3
A	166	MET	-	expression tag	UNP Q9H6W3
A	364	ALA	VAL	variant	UNP Q9H6W3
A	642	ALA	-	expression tag	UNP Q9H6W3
A	643	GLU	-	expression tag	UNP Q9H6W3
A	644	ASN	-	expression tag	UNP Q9H6W3
A	645	LEU	-	expression tag	UNP Q9H6W3
A	646	TYR	-	expression tag	UNP Q9H6W3
A	647	PHE	-	expression tag	UNP Q9H6W3
A	648	GLN	-	expression tag	UNP Q9H6W3
B	160	LEU	-	expression tag	UNP Q9H6W3
B	161	ARG	-	expression tag	UNP Q9H6W3
B	162	ARG	-	expression tag	UNP Q9H6W3
B	163	ARG	-	expression tag	UNP Q9H6W3
B	164	TYR	-	expression tag	UNP Q9H6W3
B	165	THR	-	expression tag	UNP Q9H6W3
B	166	MET	-	expression tag	UNP Q9H6W3
B	364	ALA	VAL	variant	UNP Q9H6W3
B	642	ALA	-	expression tag	UNP Q9H6W3
B	643	GLU	-	expression tag	UNP Q9H6W3

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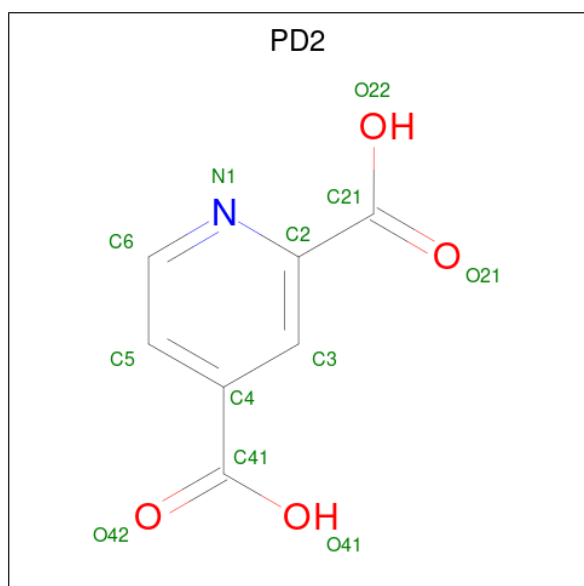
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Chain	Residue	Modelled	Actual	Comment	Reference
B	644	ASN	-	expression tag	UNP Q9H6W3
B	645	LEU	-	expression tag	UNP Q9H6W3
B	646	TYR	-	expression tag	UNP Q9H6W3
B	647	PHE	-	expression tag	UNP Q9H6W3
B	648	GLN	-	expression tag	UNP Q9H6W3

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is PYRIDINE-2,4-DICARBOXYLIC ACID (CCD ID: PD2) (formula: C₇H₅NO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 7 1 4	0	0
3	B	1	Total C N O 12 7 1 4	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

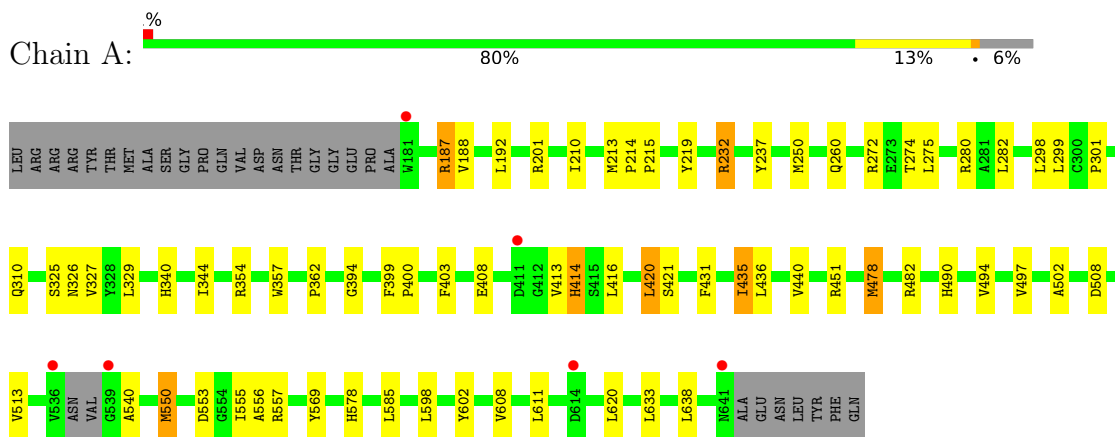
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	84	Total	O	0	0
			84	84		

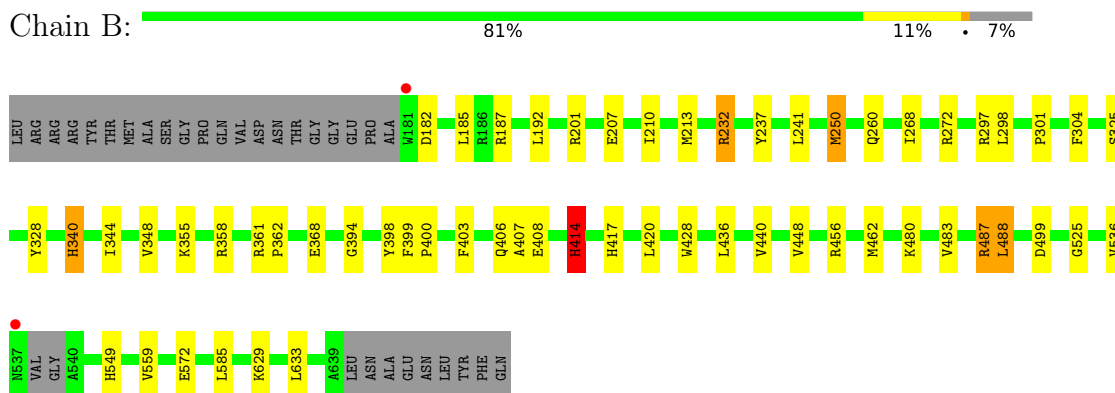
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysine-specific demethylase NO66



- Molecule 1: Lysine-specific demethylase NO66



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.67Å 149.55Å 105.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 2.40 29.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.46-2.40) 99.7 (29.46-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.185 , 0.230 0.185 , 0.231	Depositor DCC
R_{free} test set	1986 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7412	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PD2, NI, SO4

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	0.99	2/3718 (0.1%)	0.97	2/5065 (0.0%)
1	B	1.16	9/3746 (0.2%)	1.00	2/5099 (0.0%)
All	All	1.08	11/7464 (0.1%)	0.98	4/10164 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	549	HIS	ND1-CE1	7.46	1.40	1.32
1	B	549	HIS	CG-CD2	6.76	1.43	1.35
1	B	536	VAL	CA-C	5.86	1.59	1.52
1	B	428	TRP	NE1-CE2	-5.72	1.31	1.37
1	A	357	TRP	CA-C	-5.57	1.46	1.52
1	B	417	HIS	CG-CD2	5.56	1.42	1.35
1	B	525	GLY	C-O	-5.30	1.20	1.24
1	A	490	HIS	CG-CD2	5.21	1.41	1.35
1	B	398	TYR	CA-C	-5.11	1.46	1.52
1	B	414	HIS	CG-ND1	-5.02	1.32	1.38
1	B	348	VAL	N-CA	-5.01	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	VAL	N-CA-C	8.01	117.95	111.62
1	B	182	ASP	N-CA-C	5.56	119.30	107.67
1	A	299	LEU	CA-C-N	-5.36	117.39	122.37
1	A	299	LEU	C-N-CA	-5.36	117.39	122.37

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	3618	0	3495	63	0
1	B	3643	0	3544	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	3	0	0
3	B	12	0	3	1	0
4	B	5	0	0	0	0
5	A	36	0	0	1	0
5	B	84	0	0	1	0
All	All	7412	0	7045	105	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 7.

All (105) 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:550:MET:HE1	1:A:598:LEU:HB3	1.31	1.09
1:B:187[B]:ARG:HH11	1:B:187[B]:ARG:HG2	0.97	1.09
1:A:440:VAL:HG21	1:B:436:LEU:HD12	1.45	0.95
1:A:440:VAL:CG2	1:B:436:LEU:CD1	2.49	0.90
1:A:420:LEU:HD23	1:A:421:SER:N	1.86	0.90
1:B:187[B]:ARG:HG2	1:B:187[B]:ARG:NH1	1.76	0.89
1:A:250:MET:HE1	1:A:298:LEU:HD21	1.56	0.87
1:A:420:LEU:HD23	1:A:420:LEU:C	2.01	0.85
1:B:487:ARG:HH11	1:B:487:ARG:HG3	1.41	0.83
1:B:487:ARG:HH11	1:B:487:ARG:CG	1.94	0.80
1:A:431:PHE:CE2	1:A:435:ILE:CD1	2.65	0.80
1:A:440:VAL:HG21	1:B:436:LEU:CD1	2.12	0.79
1:A:280:ARG:NH1	1:A:282:LEU:HD23	1.98	0.78
1:A:440:VAL:CG2	1:B:436:LEU:HD12	2.11	0.76
1:A:431:PHE:CE2	1:A:435:ILE:HD12	2.21	0.75
1:A:344:ILE:HD12	1:A:344:ILE:O	1.87	0.75
1:B:207:GLU:OE1	5:B:814:HOH:O	2.03	0.75
1:B:344:ILE:O	1:B:344:ILE:HD12	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HD2	1:B:394:GLY:O	1.89	0.72
1:A:232:ARG:HD2	1:A:394:GLY:O	1.89	0.71
1:B:187[B]:ARG:HH11	1:B:187[B]:ARG:CG	1.86	0.71
1:A:436:LEU:HD11	1:B:488:LEU:HD21	1.73	0.70
1:A:436:LEU:HD12	1:B:440:VAL:CG2	2.24	0.68
1:A:420:LEU:C	1:A:420:LEU:CD2	2.67	0.67
1:A:440:VAL:CG2	1:B:436:LEU:HD11	2.25	0.65
1:A:502:ALA:HB1	1:A:557:ARG:HG2	1.79	0.65
1:B:344:ILE:HD12	1:B:344:ILE:C	2.22	0.64
1:A:344:ILE:HD12	1:A:344:ILE:C	2.23	0.63
1:B:420:LEU:C	1:B:420:LEU:HD23	2.24	0.63
1:A:187[A]:ARG:HG2	1:A:187[A]:ARG:HH11	1.63	0.62
1:A:232:ARG:HD3	1:A:237:TYR:CD1	2.35	0.62
1:B:232:ARG:HD3	1:B:237:TYR:CD1	2.37	0.60
1:B:480:LYS:HA	1:B:483:VAL:HG12	1.83	0.60
1:A:478:MET:O	1:A:482:ARG:HD3	2.04	0.58
1:A:187[A]:ARG:HH11	1:A:187[A]:ARG:CG	2.17	0.58
1:B:487:ARG:HG3	1:B:487:ARG:NH1	2.11	0.58
1:A:280:ARG:HH11	1:A:282:LEU:HD23	1.67	0.57
1:A:192:LEU:O	1:A:201:ARG:HD3	2.05	0.56
1:A:274:THR:C	1:A:275:LEU:HD12	2.30	0.56
1:A:508:ASP:OD1	1:A:578:HIS:NE2	2.39	0.56
1:B:572:GLU:OE2	1:B:629:LYS:NZ	2.39	0.56
1:A:440:VAL:HG22	1:B:436:LEU:HD11	1.87	0.55
1:A:280:ARG:NH1	5:A:802:HOH:O	2.38	0.55
1:A:431:PHE:HE2	1:A:435:ILE:CD1	2.15	0.55
1:B:250[B]:MET:CE	1:B:304:PHE:HB2	2.36	0.55
1:B:250[B]:MET:HE3	1:B:304:PHE:CB	2.38	0.54
1:A:540:ALA:HB3	1:A:638:LEU:O	2.07	0.54
1:A:436:LEU:HD12	1:B:440:VAL:HG21	1.89	0.54
1:A:585:LEU:C	1:A:585:LEU:HD12	2.33	0.53
1:A:550:MET:HE2	1:A:550:MET:N	2.24	0.53
1:A:232:ARG:HD3	1:A:237:TYR:CG	2.43	0.53
1:B:633:LEU:C	1:B:633:LEU:HD12	2.34	0.52
1:B:250[B]:MET:CE	1:B:298:LEU:HD21	2.41	0.51
1:B:232:ARG:HD3	1:B:237:TYR:CG	2.46	0.51
1:B:192:LEU:O	1:B:201:ARG:HD3	2.10	0.51
1:B:297:ARG:HD3	1:B:328:TYR:CE1	2.46	0.50
1:B:250[B]:MET:HE1	1:B:304:PHE:HB2	1.92	0.50
1:B:499:ASP:HB3	1:B:559:VAL:HG13	1.94	0.50
1:A:550:MET:HE2	1:A:550:MET:CA	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:C	1:A:344:ILE:CD1	2.85	0.49
1:A:219:TYR:CE1	1:B:456:ARG:HD3	2.47	0.49
1:B:344:ILE:C	1:B:344:ILE:CD1	2.85	0.48
1:B:480:LYS:HA	1:B:483:VAL:CG1	2.44	0.48
1:A:414:HIS:ND1	1:A:414:HIS:C	2.72	0.48
1:B:585:LEU:HD12	1:B:585:LEU:C	2.39	0.48
1:A:210:ILE:O	1:A:213:MET:HB3	2.15	0.47
1:B:250[B]:MET:CE	1:B:304:PHE:CB	2.93	0.47
1:B:250[B]:MET:HE3	1:B:304:PHE:CG	2.50	0.47
1:A:354:ARG:HB2	1:A:413:VAL:HG21	1.98	0.46
1:B:358:ARG:NH2	1:B:406:GLN:NE2	2.63	0.46
1:A:553:ASP:HB2	1:A:602:TYR:CE1	2.51	0.45
1:B:448:VAL:O	1:B:448:VAL:HG22	2.16	0.45
1:A:556:ALA:O	1:A:557:ARG:HD2	2.17	0.45
1:B:187[B]:ARG:NH1	1:B:187[B]:ARG:CG	2.57	0.45
1:A:362:PRO:HD3	1:A:403:PHE:CE2	2.52	0.45
1:A:633:LEU:C	1:A:633:LEU:HD12	2.41	0.45
1:B:414:HIS:ND1	1:B:414:HIS:C	2.74	0.45
1:B:487:ARG:CG	1:B:487:ARG:NH1	2.60	0.44
1:B:210:ILE:O	1:B:213:MET:HB3	2.18	0.44
1:A:436:LEU:CD1	1:B:488:LEU:HD21	2.46	0.44
1:B:362:PRO:HD3	1:B:403:PHE:CE2	2.52	0.44
1:A:550:MET:CE	1:A:598:LEU:HB3	2.22	0.44
1:A:451:ARG:NH1	1:B:368:GLU:O	2.47	0.43
1:A:435:ILE:HG13	1:A:497:VAL:HG21	2.01	0.43
1:A:310:GLN:HA	1:A:513:VAL:HG21	2.00	0.43
1:B:355:LYS:HG2	1:B:407:ALA:HB1	2.01	0.43
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.89	0.42
1:B:361:ARG:O	1:B:362:PRO:C	2.61	0.42
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.94	0.42
1:B:340:HIS:CD2	3:B:702:PD2:H6	2.54	0.42
1:A:301:PRO:HG3	1:A:327:VAL:HG23	2.00	0.42
1:B:301:PRO:HG2	1:B:325:SER:OG	2.20	0.42
1:A:555:ILE:O	1:A:569:TYR:HA	2.20	0.41
1:A:325:SER:C	1:A:326:ASN:HD22	2.27	0.41
1:A:494:VAL:CG1	1:B:462:MET:HE2	2.50	0.41
1:A:608:VAL:HG11	1:A:620:LEU:HD23	2.01	0.41
1:B:185:LEU:CD2	1:B:241:LEU:HB2	2.50	0.41
1:A:301:PRO:HG2	1:A:325:SER:OG	2.21	0.41
1:A:494:VAL:HG11	1:B:462:MET:HE2	2.01	0.41
1:B:210:ILE:HD12	1:B:213:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PHE:HA	1:B:400:PRO:HD3	1.89	0.41
1:A:275:LEU:HD12	1:A:275:LEU:N	2.35	0.40
1:A:187[B]:ARG:HH11	1:A:187[B]:ARG:HG3	1.87	0.40
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.95	0.40
1:A:329:LEU:HD13	1:A:416:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/489 (94%)	452 (99%)	5 (1%)	0	100	100
1	B	456/489 (93%)	451 (99%)	5 (1%)	0	100	100
All	All	913/978 (93%)	903 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/416 (90%)	360 (96%)	13 (4%)	32	53
1	B	381/416 (92%)	370 (97%)	11 (3%)	37	60
All	All	754/832 (91%)	730 (97%)	24 (3%)	37	56

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187[A]	ARG
1	A	187[B]	ARG
1	A	188	VAL
1	A	232	ARG
1	A	260	GLN
1	A	272	ARG
1	A	340	HIS
1	A	408	GLU
1	A	414	HIS
1	A	420	LEU
1	A	435	ILE
1	A	478	MET
1	A	550	MET
1	B	232	ARG
1	B	250[A]	MET
1	B	250[B]	MET
1	B	260	GLN
1	B	268	ILE
1	B	272	ARG
1	B	340	HIS
1	B	408	GLU
1	B	414	HIS
1	B	487	ARG
1	B	488	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	A	376	ASN
1	A	424	GLN
1	A	500	GLN
1	B	335	GLN
1	B	379	GLN
1	B	406	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	PD2	B	702	2	12,12,12	1.69	4 (33%)	16,16,16	2.09	5 (31%)
3	PD2	A	701	2	12,12,12	1.10	1 (8%)	16,16,16	2.08	6 (37%)
4	SO4	B	703	-	4,4,4	0.50	0	6,6,6	0.85	0

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	PD2	B	702	2	-	0/8/8/8	0/1/1/1
3	PD2	A	701	2	-	0/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PD2	C2-C21	-3.83	1.43	1.50
3	B	702	PD2	O42-C41	2.23	1.29	1.22
3	B	702	PD2	O41-C41	-2.07	1.24	1.30
3	B	702	PD2	O22-C21	-2.06	1.24	1.30
3	A	701	PD2	O22-C21	-2.01	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PD2	C6-N1-C2	4.40	122.60	116.93
3	B	702	PD2	O22-C21-C2	-3.81	105.67	114.71
3	B	702	PD2	C5-C4-C3	-3.66	115.02	119.25
3	B	702	PD2	O22-C21-O21	3.58	131.05	123.35
3	A	701	PD2	C5-C6-N1	-3.38	119.83	123.97
3	B	702	PD2	C6-C5-C4	3.38	122.74	119.05
3	A	701	PD2	C3-C2-N1	-3.28	119.34	123.27
3	A	701	PD2	O41-C41-C4	2.59	121.47	114.84
3	A	701	PD2	O21-C21-C2	2.58	126.49	121.30
3	A	701	PD2	C3-C2-C21	2.13	124.33	119.61
3	B	702	PD2	C5-C6-N1	-2.09	121.41	123.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	PD2	1	0

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	459/489 (93%)	-0.18	6 (1%)	75 71	19, 54, 90, 124	2 (0%)
1	B	457/489 (93%)	-0.50	2 (0%)	88 86	23, 40, 74, 104	3 (0%)
All	All	916/978 (93%)	-0.34	8 (0%)	81 78	19, 48, 85, 124	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	TRP	5.4
1	B	537	ASN	5.3
1	B	181	TRP	3.9
1	A	536	VAL	3.9
1	A	641	ASN	3.6
1	A	411	ASP	3.0
1	A	539	GLY	2.6
1	A	614	ASP	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(Å ²)	Q<0.9
4	SO4	B	703	5/5	0.88	0.08	59,72,116,161	0
3	PD2	A	701	12/12	0.95	0.08	32,46,66,79	0
3	PD2	B	702	12/12	0.98	0.05	14,23,32,42	0
2	NI	B	701	1/1	1.00	0.03	33,33,33,33	0
2	NI	A	700	1/1	1.00	0.02	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.