



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:12 PM UTC

PDB ID : 4Y33 / pdb_00004y33
Title : Crystal of NO66 in complex with Ni(II) and N-oxalylglycine (NOG)
Authors : Wang, C.; Zhang, Q.; Zang, J.
Deposited on : 2015-02-10
Resolution : 2.70 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

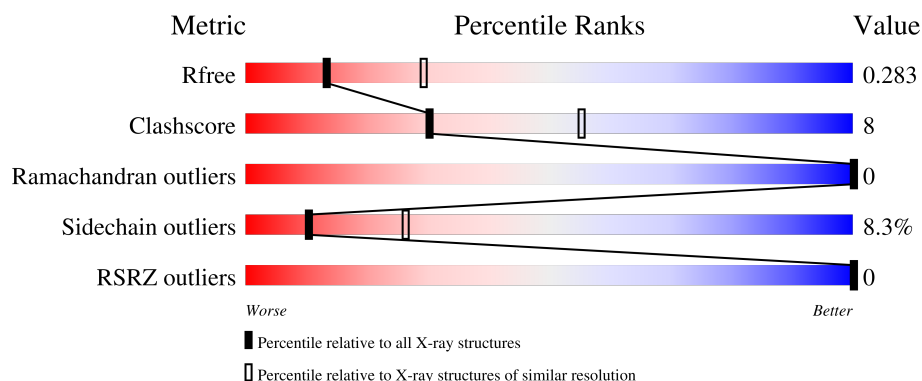
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	466	 79% 18% . .
1	B	466	 76% 20% . .
1	C	466	 74% 19% . .
1	D	466	 74% 21% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14695 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.

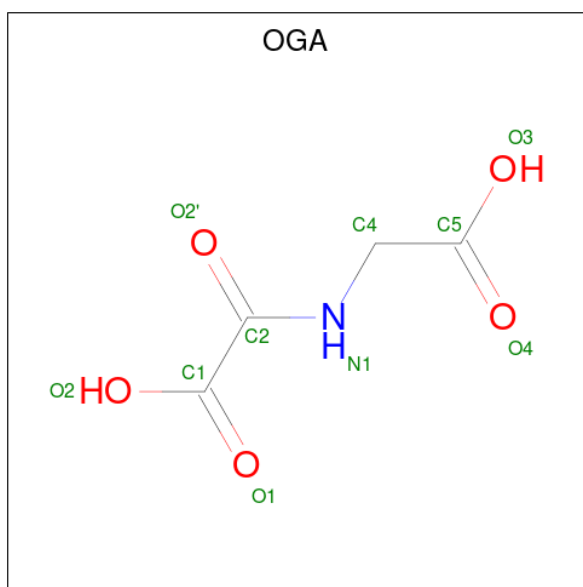
- Molecule 1 is a protein called Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3660	2327	645	673	15			
1	B	459	Total	C	N	O	S	0	0	0
			3660	2327	645	673	15			
1	C	459	Total	C	N	O	S	0	0	0
			3660	2327	645	673	15			
1	D	459	Total	C	N	O	S	0	2	0
			3676	2337	651	673	15			

- 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		
2	C	1	Total	Ni	0	0
			1	1		
2	D	1	Total	Ni	0	0
			1	1		

- Molecule 3 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	4	1	5		
3	B	1	Total	C	N	O	0	0
			10	4	1	5		
3	C	1	Total	C	N	O	0	0
			10	4	1	5		

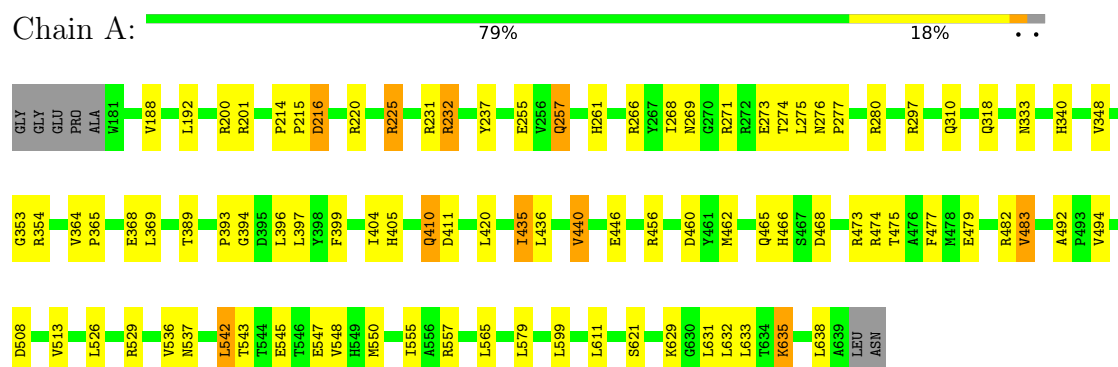
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		

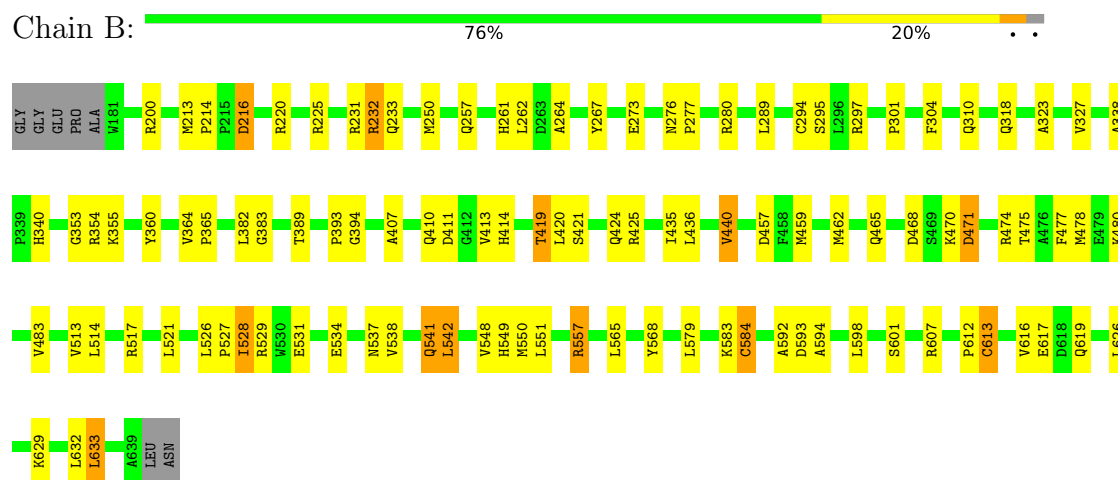
3 Residue-property plots

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.

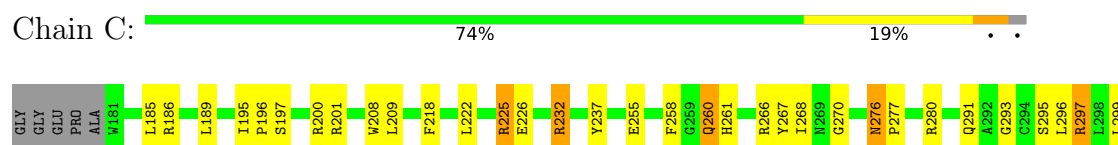
- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66

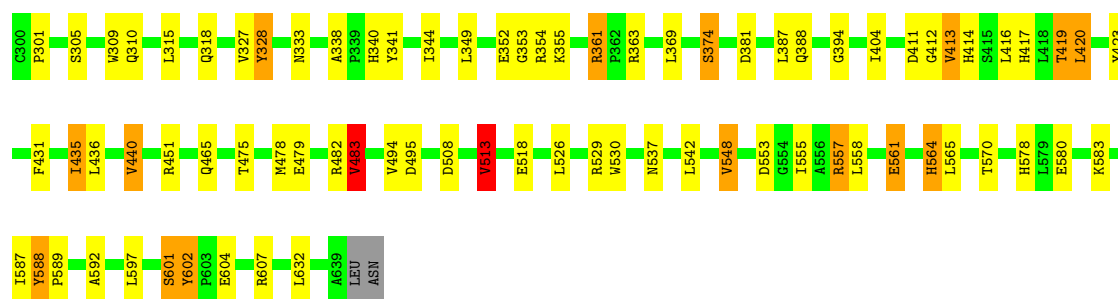


- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66



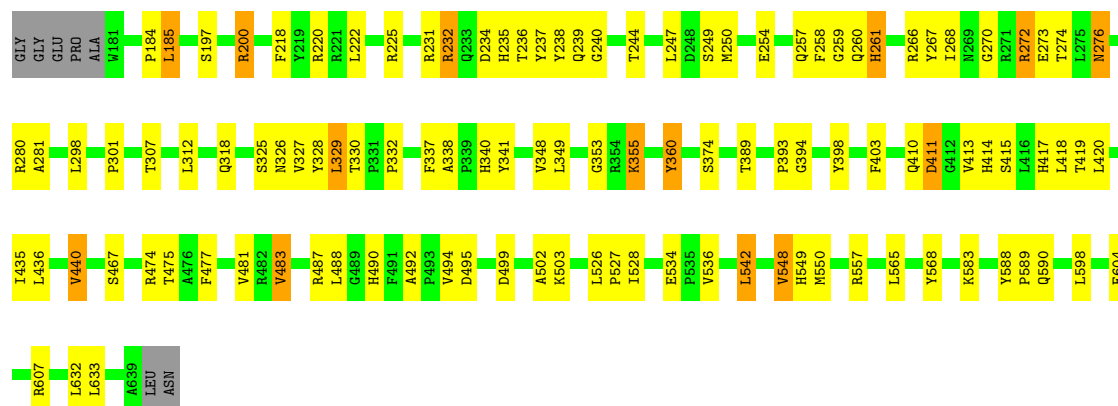
- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66





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

Chain D: 74% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.59Å 150.88Å 106.90Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	38.89 – 2.70 38.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.89-2.70) 97.5 (38.89-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.233 , 0.274 (Not available) , 0.283	Depositor DCC
R_{free} test set	3562 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14695	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: NI, OGA

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	1.11	3/3755 (0.1%)	1.10	14/5113 (0.3%)
1	B	1.06	2/3755 (0.1%)	1.10	15/5113 (0.3%)
1	C	0.92	0/3755	1.07	14/5113 (0.3%)
1	D	0.90	0/3771	1.11	15/5133 (0.3%)
All	All	1.00	5/15036 (0.0%)	1.09	58/20472 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	HIS	C-O	-6.89	1.16	1.23
1	B	262	LEU	C-O	-5.35	1.18	1.23
1	B	633	LEU	C-O	-5.24	1.17	1.23
1	A	599	LEU	C-O	-5.17	1.18	1.24
1	A	225	ARG	C-O	-5.04	1.17	1.24

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	GLN	N-CA-C	-15.75	91.02	112.12
1	C	413	VAL	N-CA-CB	11.83	128.44	111.05
1	C	412	GLY	N-CA-C	9.25	129.33	115.08
1	D	234	ASP	CB-CA-C	8.97	126.58	110.16
1	D	235	HIS	N-CA-C	-8.93	101.70	114.12
1	D	234	ASP	N-CA-C	-8.77	94.90	108.76
1	A	440	VAL	CB-CA-C	-8.11	101.51	111.88
1	D	411	ASP	CB-CA-C	-7.54	98.99	111.51
1	A	277	PRO	CA-C-N	-7.53	112.57	120.03
1	A	277	PRO	C-N-CA	-7.53	112.57	120.03
1	D	259	GLY	N-CA-C	7.46	125.44	115.59
1	C	277	PRO	CA-C-N	-7.38	112.40	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	PRO	C-N-CA	-7.38	112.40	119.85
1	B	440	VAL	CB-CA-C	-7.22	101.50	112.05
1	B	613	CYS	N-CA-CB	7.04	122.44	111.24
1	B	276	ASN	CA-C-N	-6.95	114.59	119.66
1	B	276	ASN	C-N-CA	-6.95	114.59	119.66
1	A	276	ASN	CA-C-N	-6.92	114.68	119.66
1	A	276	ASN	C-N-CA	-6.92	114.68	119.66
1	A	611	LEU	CA-C-N	6.83	128.38	119.84
1	A	611	LEU	C-N-CA	6.83	128.38	119.84
1	A	410	GLN	N-CA-C	6.82	121.25	112.12
1	B	471	ASP	CA-C-N	6.70	126.38	119.82
1	B	471	ASP	C-N-CA	6.70	126.38	119.82
1	C	440	VAL	CB-CA-C	-6.49	103.27	112.22
1	B	541	GLN	N-CA-C	-6.09	102.68	110.53
1	A	473	ARG	N-CA-C	-5.85	106.69	113.88
1	D	440	VAL	CB-CA-C	-5.81	103.16	112.16
1	D	260	GLN	N-CA-CB	5.80	121.89	110.63
1	B	478	MET	CB-CA-C	-5.70	99.40	110.46
1	A	508	ASP	N-CA-C	5.70	118.26	111.71
1	C	276	ASN	CA-C-N	-5.70	115.56	119.66
1	C	276	ASN	C-N-CA	-5.70	115.56	119.66
1	A	271	ARG	N-CA-C	5.58	117.52	108.26
1	C	513	VAL	CB-CA-C	-5.52	103.42	110.98
1	B	480	LYS	N-CA-C	5.52	117.29	111.28
1	D	477	PHE	N-CA-C	-5.46	105.22	111.07
1	D	527	PRO	CB-CA-C	-5.41	103.94	110.00
1	D	235	HIS	N-CA-CB	5.40	118.33	110.88
1	C	431	PHE	N-CA-C	-5.40	105.30	111.07
1	B	592	ALA	N-CA-C	5.39	117.16	111.28
1	D	481	VAL	N-CA-C	-5.38	105.25	110.42
1	C	260	GLN	N-CA-C	-5.35	105.02	112.45
1	B	277	PRO	CA-C-N	-5.27	114.56	120.14
1	B	277	PRO	C-N-CA	-5.27	114.56	120.14
1	C	374	SER	CA-C-N	-5.26	115.16	120.21
1	C	374	SER	C-N-CA	-5.26	115.16	120.21
1	A	399	PHE	CA-C-N	5.24	125.21	120.03
1	A	399	PHE	C-N-CA	5.24	125.21	120.03
1	D	483	VAL	N-CA-CB	5.23	117.27	110.57
1	C	483	VAL	N-CA-CB	5.20	118.38	110.58
1	C	570	THR	CB-CA-C	-5.15	101.03	109.99
1	B	528	ILE	N-CA-C	5.10	115.82	108.93
1	D	261	HIS	N-CA-C	5.10	120.15	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	584	CYS	N-CA-C	5.07	116.00	108.60
1	D	534	GLU	N-CA-C	5.06	112.57	108.07
1	A	257	GLN	CB-CA-C	-5.01	101.03	109.50
1	B	383	GLY	N-CA-C	-5.01	105.42	112.13

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	3660	0	3556	55	0
1	B	3660	0	3556	67	0
1	C	3660	0	3556	70	0
1	D	3676	0	3576	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	3	0	0
3	B	10	0	3	1	0
3	C	10	0	3	2	0
4	A	5	0	0	0	0
All	All	14695	0	14253	243	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 8.

All (243) 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:479:GLU:OE1	1:A:482:ARG:NH1	1.86	1.08
1:D:487[B]:ARG:HD2	1:D:487[B]:ARG:O	1.63	0.96
1:D:254:GLU:O	1:D:280:ARG:NH2	2.04	0.91
1:B:462:MET:HE2	1:B:477:PHE:CG	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ARG:O	1:C:361:ARG:NH2	2.12	0.82
1:B:462:MET:CE	1:B:477:PHE:CD2	2.63	0.81
1:D:328:TYR:CE1	1:D:337:PHE:HE2	1.99	0.81
1:B:542:LEU:HD23	1:B:542:LEU:H	1.46	0.81
1:A:548:VAL:CG2	1:A:632:LEU:HG	2.12	0.78
1:B:462:MET:HE2	1:B:477:PHE:CD2	2.18	0.77
1:D:266:ARG:HD2	1:D:268:ILE:HD11	1.68	0.75
1:C:232:ARG:HD2	1:C:394:GLY:O	1.88	0.74
1:B:548:VAL:CG2	1:B:632:LEU:HG	2.17	0.73
1:C:597:LEU:O	1:C:601:SER:OG	2.05	0.73
1:C:419:THR:HG21	3:C:702:OGA:O1	1.91	0.70
1:A:548:VAL:HG23	1:A:632:LEU:HG	1.73	0.70
1:B:338:ALA:O	1:B:340:HIS:HD2	1.74	0.70
1:A:257:GLN:H	1:A:261:HIS:HD2	1.42	0.68
1:C:353:GLY:HA3	1:C:414:HIS:O	1.94	0.67
1:D:218:PHE:HA	1:D:222:LEU:HD12	1.78	0.66
1:D:328:TYR:CD1	1:D:337:PHE:HE2	2.14	0.65
1:A:232:ARG:HD2	1:A:394:GLY:O	1.96	0.64
1:C:333:ASN:HD21	1:C:411:ASP:HA	1.62	0.64
1:D:353:GLY:HA3	1:D:414:HIS:O	1.99	0.63
1:D:353:GLY:O	1:D:393:PRO:HD3	1.99	0.63
1:D:328:TYR:CE1	1:D:337:PHE:CE2	2.85	0.62
1:D:338:ALA:O	1:D:340:HIS:HD2	1.82	0.62
1:D:550:MET:HE3	1:D:598:LEU:HB3	1.82	0.61
1:D:328:TYR:HE1	1:D:337:PHE:CE2	2.19	0.61
1:B:527:PRO:HB2	1:B:537:ASN:HD22	1.64	0.61
1:A:274:THR:C	1:A:275:LEU:HD12	2.26	0.61
1:B:440:VAL:HG21	1:D:436:LEU:HD12	1.82	0.60
1:B:548:VAL:HG23	1:B:632:LEU:HG	1.84	0.60
1:A:548:VAL:HG21	1:A:632:LEU:HD21	1.84	0.60
1:D:185:LEU:HD23	1:D:239:GLN:O	2.02	0.60
1:B:462:MET:HE2	1:B:477:PHE:HB3	1.84	0.59
1:D:329:LEU:C	1:D:329:LEU:HD12	2.27	0.59
1:C:232:ARG:CD	1:C:394:GLY:O	2.50	0.59
1:C:435:ILE:HD11	1:C:494:VAL:HA	1.83	0.59
1:C:548:VAL:HG23	1:C:632:LEU:HG	1.83	0.59
1:A:548:VAL:CG2	1:A:632:LEU:CG	2.79	0.59
1:A:548:VAL:HG21	1:A:632:LEU:CG	2.34	0.58
1:B:462:MET:HE3	1:B:477:PHE:CD2	2.39	0.58
1:D:312:LEU:HD11	1:D:325:SER:OG	2.04	0.57
1:B:550:MET:HE3	1:B:598:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:TYR:CE2	1:C:374:SER:HB3	2.39	0.57
1:A:354:ARG:HH11	1:A:354:ARG:HG3	1.70	0.56
1:C:301:PRO:HG3	1:C:327:VAL:HG23	1.87	0.56
1:A:333:ASN:ND2	1:A:410:GLN:O	2.38	0.56
1:B:462:MET:HE2	1:B:477:PHE:CB	2.35	0.56
1:C:226:GLU:OE1	1:C:226:GLU:HA	2.06	0.56
1:A:435:ILE:HD11	1:A:494:VAL:HA	1.87	0.56
1:A:436:LEU:CD1	1:C:440:VAL:CG2	2.83	0.56
1:A:436:LEU:HD12	1:C:440:VAL:HG21	1.87	0.56
1:B:548:VAL:HG21	1:B:632:LEU:CG	2.36	0.56
1:B:528:ILE:HD12	1:B:538:VAL:HA	1.88	0.55
1:D:257:GLN:H	1:D:261:HIS:HD2	1.55	0.55
1:D:258:PHE:HB3	1:D:276:ASN:HB3	1.88	0.55
1:B:436:LEU:HD12	1:D:440:VAL:CG2	2.36	0.55
1:B:542:LEU:HD23	1:B:542:LEU:N	2.17	0.55
1:B:557:ARG:HH11	1:B:557:ARG:HG2	1.72	0.54
1:A:548:VAL:HG21	1:A:632:LEU:CD2	2.37	0.54
1:B:474:ARG:NH2	1:D:495:ASP:OD2	2.29	0.54
1:B:257:GLN:H	1:B:261:HIS:HD2	1.55	0.54
1:B:550:MET:HE1	1:B:626:LEU:HD13	1.89	0.54
1:C:260:GLN:HG2	1:C:261:HIS:CE1	2.43	0.54
1:C:548:VAL:CG2	1:C:632:LEU:HD11	2.38	0.53
1:D:435:ILE:HD11	1:D:494:VAL:HA	1.89	0.53
1:B:436:LEU:HD11	1:D:488:LEU:CD1	2.38	0.53
1:D:502:ALA:HB1	1:D:557:ARG:HG2	1.91	0.53
1:C:208:TRP:CZ2	1:C:237:TYR:CE1	2.96	0.53
1:A:456:ARG:HA	1:C:423:TYR:OH	2.09	0.52
1:A:436:LEU:CD1	1:C:440:VAL:HG21	2.40	0.52
1:B:548:VAL:CG2	1:B:632:LEU:CG	2.87	0.52
1:B:548:VAL:HG21	1:B:632:LEU:HD21	1.89	0.52
1:D:298:LEU:O	1:D:301:PRO:HD3	2.09	0.52
1:D:349:LEU:HD12	1:D:349:LEU:N	2.25	0.52
1:A:474:ARG:NH2	1:C:495:ASP:OD2	2.36	0.52
1:C:295:SER:O	1:C:296:LEU:HD23	2.10	0.52
1:B:548:VAL:HG21	1:B:632:LEU:CD2	2.40	0.51
1:D:266:ARG:O	1:D:272:ARG:HA	2.10	0.51
1:C:195:ILE:O	1:C:201:ARG:NH1	2.43	0.51
1:C:341:TYR:CZ	1:C:374:SER:HB3	2.45	0.51
1:B:548:VAL:HG21	1:B:632:LEU:HG	1.92	0.51
1:B:301:PRO:HG3	1:B:327:VAL:HG23	1.92	0.50
1:B:612:PRO:O	1:B:613:CYS:SG	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:548:VAL:HG21	1:D:632:LEU:HD11	1.93	0.50
1:A:550:MET:HE2	1:A:632:LEU:CD1	2.40	0.50
1:A:368:GLU:O	1:C:451:ARG:NH1	2.40	0.50
1:B:232:ARG:HD2	1:B:394:GLY:O	2.12	0.50
1:C:349:LEU:N	1:C:349:LEU:HD12	2.26	0.50
1:D:257:GLN:H	1:D:261:HIS:CD2	2.30	0.50
1:D:542:LEU:HD23	1:D:542:LEU:H	1.77	0.50
1:A:188:VAL:O	1:A:192:LEU:HG	2.12	0.50
1:A:231:ARG:NH2	1:A:389:THR:OG1	2.44	0.49
1:B:440:VAL:CG2	1:D:436:LEU:CD1	2.90	0.49
1:C:508:ASP:OD1	1:C:578:HIS:NE2	2.43	0.49
1:D:355[A]:LYS:HD3	1:D:415:SER:CB	2.41	0.49
1:B:550:MET:HE2	1:B:632:LEU:CD1	2.42	0.49
1:A:474:ARG:HH22	1:C:495:ASP:CG	2.20	0.49
1:A:435:ILE:HD12	1:A:492:ALA:HB1	1.95	0.49
1:B:517:ARG:HG2	1:B:521:LEU:HD12	1.93	0.49
1:A:529:ARG:NH1	1:A:537:ASN:ND2	2.60	0.49
1:A:542:LEU:HD22	1:A:638:LEU:HD11	1.95	0.49
1:D:360:TYR:N	1:D:360:TYR:CD2	2.81	0.49
1:D:398:TYR:CD2	1:D:398:TYR:C	2.90	0.49
1:A:440:VAL:CG2	1:C:436:LEU:CD1	2.91	0.49
1:A:555:ILE:HD12	1:A:631:LEU:HD23	1.95	0.48
1:C:557:ARG:HG3	1:C:557:ARG:HH11	1.78	0.48
1:D:184:PRO:HD2	1:D:236:THR:O	2.14	0.48
1:A:257:GLN:H	1:A:261:HIS:CD2	2.28	0.48
1:A:275:LEU:HD12	1:A:275:LEU:N	2.29	0.48
1:B:529:ARG:HH12	1:B:537:ASN:ND2	2.11	0.48
1:D:548:VAL:CG2	1:D:632:LEU:HD11	2.44	0.48
1:B:419:THR:HG21	3:B:702:OGA:O2	2.14	0.48
1:B:257:GLN:H	1:B:261:HIS:CD2	2.32	0.48
1:C:561:GLU:O	1:C:564:HIS:HB2	2.13	0.48
1:D:338:ALA:O	1:D:340:HIS:CD2	2.65	0.48
1:C:266:ARG:HG2	1:C:293:GLY:O	2.14	0.47
1:A:232:ARG:CD	1:A:394:GLY:O	2.63	0.47
1:B:360:TYR:CZ	1:B:382:LEU:HD13	2.49	0.47
1:C:315:LEU:CD1	1:C:420:LEU:HD11	2.44	0.47
1:B:216:ASP:OD1	1:B:220:ARG:NH2	2.46	0.47
1:B:514:LEU:HD21	1:B:551:LEU:HD21	1.97	0.47
1:C:297:ARG:HE	1:C:299:LEU:CD2	2.28	0.47
1:A:579:LEU:O	1:A:579:LEU:HD23	2.15	0.47
1:C:310:GLN:HA	1:C:513:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD23	1:D:238:TYR:C	2.40	0.47
1:C:267:TYR:OH	1:C:270:GLY:HA2	2.13	0.47
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.80	0.46
1:D:499:ASP:OD1	1:D:557:ARG:NH1	2.37	0.46
1:D:185:LEU:CD2	1:D:238:TYR:C	2.88	0.46
1:B:633:LEU:HD12	1:B:633:LEU:C	2.39	0.46
1:C:529:ARG:HH12	1:C:537:ASN:ND2	2.13	0.46
1:C:338:ALA:O	1:C:340:HIS:HD2	1.99	0.46
1:D:487[B]:ARG:NH2	1:D:490:HIS:CG	2.84	0.46
1:B:355:LYS:HG2	1:B:407:ALA:HB1	1.98	0.46
1:D:280:ARG:NH1	1:D:281:ALA:O	2.49	0.46
1:B:231:ARG:NH2	1:B:389:THR:OG1	2.49	0.45
1:B:436:LEU:HD12	1:D:440:VAL:HG22	1.98	0.45
1:D:240:GLY:O	1:D:307:THR:HG21	2.17	0.45
1:D:467:SER:HA	1:D:474:ARG:NH2	2.31	0.45
1:D:588:TYR:HB3	1:D:589:PRO:HD2	1.97	0.45
1:D:185:LEU:HD23	1:D:239:GLN:C	2.41	0.45
1:D:418:LEU:C	1:D:418:LEU:HD23	2.42	0.45
1:C:185:LEU:O	1:C:189:LEU:HG	2.17	0.45
1:D:528:ILE:HA	1:D:536:VAL:O	2.17	0.45
1:B:440:VAL:CG2	1:D:436:LEU:HD12	2.47	0.45
1:D:231:ARG:NH2	1:D:389:THR:OG1	2.49	0.45
1:D:435:ILE:HD12	1:D:492:ALA:HB1	1.99	0.45
1:C:363:ARG:HH12	1:C:381:ASP:HB3	1.82	0.45
1:D:325:SER:C	1:D:326:ASN:HD22	2.24	0.45
1:B:568:TYR:CD1	1:B:584:CYS:HB3	2.52	0.45
1:C:266:ARG:HD2	1:C:268:ILE:HD11	1.99	0.45
1:C:267:TYR:CE1	1:C:338:ALA:HB2	2.52	0.45
1:A:536:VAL:HG23	1:A:537:ASN:ND2	2.32	0.44
1:A:543:THR:C	1:A:545:GLU:H	2.25	0.44
1:C:352:GLU:HB2	1:C:416:LEU:HB3	1.98	0.44
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.79	0.44
1:C:195:ILE:HA	1:C:196:PRO:HD3	1.87	0.44
1:C:548:VAL:HG21	1:C:632:LEU:HD21	1.99	0.44
1:D:301:PRO:HG3	1:D:327:VAL:HG23	1.99	0.44
1:D:503:LYS:HD2	1:D:568:TYR:CZ	2.53	0.44
1:A:232:ARG:HD3	1:A:237:TYR:CD1	2.53	0.44
1:A:479:GLU:O	1:A:483:VAL:HG12	2.18	0.44
1:C:218:PHE:HA	1:C:222:LEU:HD12	2.00	0.44
1:C:417:HIS:HE1	3:C:702:OGA:O4	2.01	0.44
1:C:553:ASP:HB2	1:C:602:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:LEU:HD11	1:C:587:ILE:HG13	2.00	0.44
1:B:289:LEU:O	1:B:294:CYS:HB2	2.18	0.44
1:B:424:GLN:O	1:B:425:ARG:C	2.61	0.44
1:A:364:VAL:O	1:A:365:PRO:C	2.60	0.43
1:C:185:LEU:HD11	1:C:189:LEU:HD11	2.00	0.43
1:D:232:ARG:CD	1:D:394:GLY:O	2.66	0.43
1:A:479:GLU:O	1:A:483:VAL:CG1	2.66	0.43
1:D:436:LEU:O	1:D:440:VAL:HG23	2.18	0.43
1:A:462:MET:HE2	1:A:477:PHE:CD2	2.54	0.43
1:C:258:PHE:HB3	1:C:276:ASN:HB3	1.99	0.43
1:C:588:TYR:N	1:C:588:TYR:CD1	2.87	0.43
1:A:550:MET:HE2	1:A:632:LEU:HD13	2.00	0.43
1:B:353:GLY:O	1:B:393:PRO:HD3	2.18	0.43
1:C:341:TYR:CD1	1:C:341:TYR:C	2.97	0.43
1:A:266:ARG:HD2	1:A:268:ILE:HD11	2.00	0.43
1:B:264:ALA:HA	1:B:295:SER:O	2.19	0.43
1:C:209:LEU:C	1:C:232:ARG:HH22	2.25	0.43
1:A:440:VAL:HG21	1:C:436:LEU:HD12	2.01	0.43
1:C:369:LEU:HD23	1:C:369:LEU:HA	1.91	0.43
1:D:348:VAL:HG13	1:D:417:HIS:CD2	2.54	0.43
1:A:460:ASP:O	1:A:466:HIS:CE1	2.72	0.42
1:C:478:MET:O	1:C:482:ARG:HG3	2.19	0.42
1:D:341:TYR:CZ	1:D:374:SER:HB3	2.54	0.42
1:D:549:HIS:CE1	1:D:633:LEU:HD11	2.55	0.42
1:A:192:LEU:O	1:A:201:ARG:HD3	2.19	0.42
1:B:594:ALA:HB2	1:B:612:PRO:O	2.19	0.42
1:C:530:TRP:CE2	1:D:244:THR:HG21	2.54	0.42
1:B:364:VAL:O	1:B:365:PRO:C	2.62	0.42
1:C:315:LEU:HD13	1:C:420:LEU:HD11	2.01	0.42
1:B:529:ARG:NH1	1:B:537:ASN:ND2	2.66	0.42
1:A:404:ILE:HG22	1:A:405:HIS:N	2.33	0.42
1:D:232:ARG:HD3	1:D:237:TYR:CD1	2.54	0.42
1:B:353:GLY:HA3	1:B:414:HIS:O	2.20	0.42
1:D:633:LEU:HD12	1:D:633:LEU:C	2.45	0.42
1:A:310:GLN:HA	1:A:513:VAL:HG21	2.02	0.42
1:A:633:LEU:C	1:A:633:LEU:HD12	2.44	0.42
1:B:310:GLN:HA	1:B:513:VAL:HG21	2.00	0.42
1:B:542:LEU:N	1:B:542:LEU:CD2	2.83	0.42
1:B:470:LYS:O	1:B:471:ASP:C	2.62	0.42
1:B:633:LEU:HD12	1:B:633:LEU:O	2.20	0.41
1:C:589:PRO:HA	1:C:592:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PRO:HD3	1:D:414:HIS:HB3	2.02	0.41
1:B:549:HIS:CE1	1:B:633:LEU:HD11	2.56	0.41
1:C:208:TRP:CE2	1:C:237:TYR:CE1	3.09	0.41
1:C:479:GLU:O	1:C:483:VAL:HG13	2.20	0.41
1:A:268:ILE:HG22	1:A:269:ASN:N	2.35	0.41
1:C:557:ARG:HH11	1:C:557:ARG:CG	2.32	0.41
1:A:216:ASP:OD1	1:A:220:ARG:NH2	2.54	0.41
1:A:369:LEU:O	1:C:451:ARG:HD2	2.19	0.41
1:D:341:TYR:CE2	1:D:374:SER:HB3	2.56	0.41
1:B:323:ALA:HA	1:B:421:SER:O	2.21	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.99	0.41
1:B:616:VAL:O	1:B:619:GLN:HB2	2.21	0.41
1:D:360:TYR:O	1:D:403:PHE:CD1	2.74	0.41
1:D:633:LEU:HD12	1:D:633:LEU:O	2.20	0.41
1:A:348:VAL:HB	1:A:397:LEU:HB3	2.03	0.41
1:B:579:LEU:HD23	1:B:579:LEU:O	2.20	0.41
1:A:353:GLY:O	1:A:393:PRO:HD3	2.21	0.41
1:A:547:GLU:HB2	1:A:635:LYS:HB2	2.02	0.41
1:B:250:MET:HE2	1:B:304:PHE:HB2	2.02	0.41
1:C:201:ARG:NH2	1:C:518:GLU:OE2	2.46	0.41
1:C:548:VAL:HG21	1:C:632:LEU:HD11	2.02	0.41
1:D:267:TYR:CZ	1:D:270:GLY:HA2	2.56	0.41
1:A:440:VAL:HG21	1:C:436:LEU:CD1	2.51	0.41
1:C:297:ARG:HD3	1:C:328:TYR:CE1	2.56	0.40
1:C:588:TYR:N	1:C:588:TYR:HD1	2.19	0.40
1:B:457:ASP:OD1	1:B:457:ASP:N	2.54	0.40
1:B:213:MET:HA	1:B:214:PRO:HD3	1.95	0.40
1:C:387:LEU:HD23	1:C:388:GLN:N	2.36	0.40
1:D:247:LEU:O	1:D:250:MET:HB3	2.21	0.40
1:B:232:ARG:CD	1:B:394:GLY:O	2.69	0.40
1:B:267:TYR:CE1	1:B:338:ALA:HB2	2.56	0.40
1:C:309:TRP:O	1:C:309:TRP:CD1	2.75	0.40
1:D:197:SER:HB3	1:D:200:ARG:HB2	2.03	0.40
1:D:258:PHE:CE2	1:D:281:ALA:HA	2.56	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	457/466 (98%)	442 (97%)	15 (3%)	0	100	100
1	B	457/466 (98%)	449 (98%)	8 (2%)	0	100	100
1	C	457/466 (98%)	434 (95%)	23 (5%)	0	100	100
1	D	459/466 (98%)	439 (96%)	20 (4%)	0	100	100
All	All	1830/1864 (98%)	1764 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	386/397 (97%)	361 (94%)	25 (6%)	15	37
1	B	386/397 (97%)	353 (92%)	33 (8%)	10	25
1	C	386/397 (97%)	346 (90%)	40 (10%)	7	17
1	D	387/397 (98%)	356 (92%)	31 (8%)	11	28
All	All	1545/1588 (97%)	1416 (92%)	129 (8%)	10	26

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	216	ASP

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	232	ARG
1	A	255	GLU
1	A	273	GLU
1	A	280	ARG
1	A	297	ARG
1	A	318	GLN
1	A	396	LEU
1	A	411	ASP
1	A	420	LEU
1	A	435	ILE
1	A	446	GLU
1	A	465	GLN
1	A	468	ASP
1	A	475	THR
1	A	483	VAL
1	A	526	LEU
1	A	542	LEU
1	A	557	ARG
1	A	565	LEU
1	A	621	SER
1	A	629	LYS
1	A	635	LYS
1	B	200	ARG
1	B	216	ASP
1	B	225	ARG
1	B	232	ARG
1	B	233	GLN
1	B	273	GLU
1	B	280	ARG
1	B	297	ARG
1	B	318	GLN
1	B	410	GLN
1	B	411	ASP
1	B	413	VAL
1	B	419	THR
1	B	420	LEU
1	B	435	ILE
1	B	459	MET
1	B	465	GLN
1	B	468	ASP
1	B	475	THR

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Mol	Chain	Res	Type
1	B	483	VAL
1	B	526	LEU
1	B	531	GLU
1	B	534	GLU
1	B	541	GLN
1	B	542	LEU
1	B	557	ARG
1	B	565	LEU
1	B	583	LYS
1	B	593	ASP
1	B	601	SER
1	B	607	ARG
1	B	617	GLU
1	B	629	LYS
1	C	186	ARG
1	C	197	SER
1	C	200	ARG
1	C	225	ARG
1	C	232	ARG
1	C	255	GLU
1	C	280	ARG
1	C	291	GLN
1	C	297	ARG
1	C	305	SER
1	C	318	GLN
1	C	328	TYR
1	C	344	ILE
1	C	354	ARG
1	C	355	LYS
1	C	361	ARG
1	C	404	ILE
1	C	413	VAL
1	C	419	THR
1	C	420	LEU
1	C	435	ILE
1	C	465	GLN
1	C	475	THR
1	C	483	VAL
1	C	513	VAL
1	C	526	LEU
1	C	542	LEU
1	C	548	VAL

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Mol	Chain	Res	Type
1	C	555	ILE
1	C	557	ARG
1	C	561	GLU
1	C	564	HIS
1	C	565	LEU
1	C	580	GLU
1	C	583	LYS
1	C	588	TYR
1	C	601	SER
1	C	602	TYR
1	C	604	GLU
1	C	607	ARG
1	D	185	LEU
1	D	200	ARG
1	D	220	ARG
1	D	225	ARG
1	D	232	ARG
1	D	249	SER
1	D	272	ARG
1	D	273	GLU
1	D	274	THR
1	D	276	ASN
1	D	318	GLN
1	D	329	LEU
1	D	330	THR
1	D	355[A]	LYS
1	D	355[B]	LYS
1	D	360	TYR
1	D	410	GLN
1	D	411	ASP
1	D	413	VAL
1	D	419	THR
1	D	420	LEU
1	D	475	THR
1	D	483	VAL
1	D	526	LEU
1	D	542	LEU
1	D	548	VAL
1	D	565	LEU
1	D	583	LYS
1	D	590	GLN
1	D	604	GLU

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Mol	Chain	Res	Type
1	D	607	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	291	GLN
1	A	310	GLN
1	A	318	GLN
1	A	333	ASN
1	A	414	HIS
1	A	447	ASN
1	A	466	HIS
1	A	537	ASN
1	A	590	GLN
1	B	217	HIS
1	B	261	HIS
1	B	333	ASN
1	B	340	HIS
1	B	388	GLN
1	B	414	HIS
1	B	500	GLN
1	B	537	ASN
1	B	590	GLN
1	C	261	HIS
1	C	318	GLN
1	C	326	ASN
1	C	333	ASN
1	C	340	HIS
1	C	406	GLN
1	C	410	GLN
1	D	318	GLN
1	D	326	ASN
1	D	333	ASN
1	D	340	HIS
1	D	410	GLN
1	D	414	HIS
1	D	590	GLN
1	D	591	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 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	OGA	C	702	2	9,9,9	2.09	2 (22%)	8,11,11	1.47	2 (25%)
3	OGA	A	702	2	9,9,9	1.71	1 (11%)	8,11,11	1.32	2 (25%)
3	OGA	B	702	2	9,9,9	2.54	2 (22%)	8,11,11	1.27	1 (12%)

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	OGA	C	702	2	-	0/8/9/9	-
3	OGA	A	702	2	-	0/8/9/9	-
3	OGA	B	702	2	-	0/8/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	OGA	C2-C1	-6.69	1.46	1.54
3	C	702	OGA	C2-C1	-5.30	1.48	1.54
3	A	702	OGA	C2-C1	-4.29	1.49	1.54
3	C	702	OGA	O2-C1	-2.30	1.24	1.30
3	B	702	OGA	O2-C1	-2.07	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	OGA	O2'-C2-N1	-2.61	118.64	123.35
3	C	702	OGA	O2-C1-O1	-2.44	118.09	123.90
3	C	702	OGA	O2'-C2-N1	-2.43	118.97	123.35
3	A	702	OGA	O2-C1-O1	-2.24	118.56	123.90
3	B	702	OGA	O2'-C2-C1	-2.14	118.54	121.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	OGA	2	0
3	B	702	OGA	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	459/466 (98%)	-1.61	0 100 100	11, 25, 49, 76	1 (0%)
1	B	459/466 (98%)	-1.59	0 100 100	12, 26, 52, 68	1 (0%)
1	C	459/466 (98%)	-1.32	0 100 100	13, 44, 76, 103	1 (0%)
1	D	459/466 (98%)	-1.26	0 100 100	10, 50, 79, 107	3 (0%)
All	All	1836/1864 (98%)	-1.44	0 100 100	10, 36, 70, 107	6 (0%)

There are no RSRZ outliers to report.

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
2	NI	A	701	1/1	0.99	0.02	61,61,61,61	0
2	NI	C	701	1/1	0.99	0.04	74,74,74,74	0
2	NI	D	701	1/1	0.99	0.02	77,77,77,77	0
3	OGA	A	702	10/10	0.99	0.04	23,24,32,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OGA	B	702	10/10	0.99	0.06	26,27,40,44	0
3	OGA	C	702	10/10	0.99	0.06	43,53,77,86	0
2	NI	B	701	1/1	1.00	0.01	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.