



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:13 am GMT

PDB ID : 4Y33  
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](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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

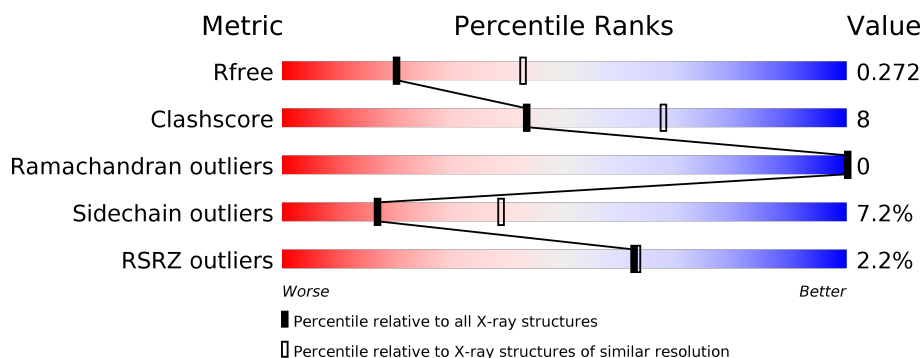
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 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	466	<div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
1	B	466	<div> <div>%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	C	466	<div> <div>3%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
1	D	466	<div> <div>5%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OGA	C	702	-	-	-	X

## 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.

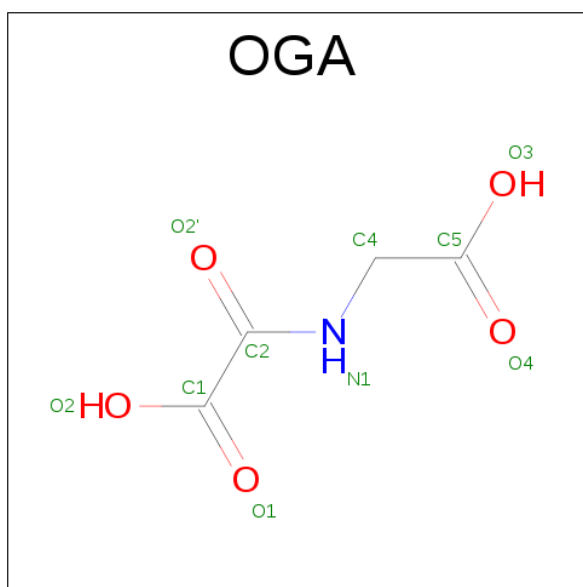
- Molecule 1 is a protein called Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66.

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 (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		
2	D	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		

- Molecule 3 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C<sub>4</sub>H<sub>5</sub>NO<sub>5</sub>).



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		

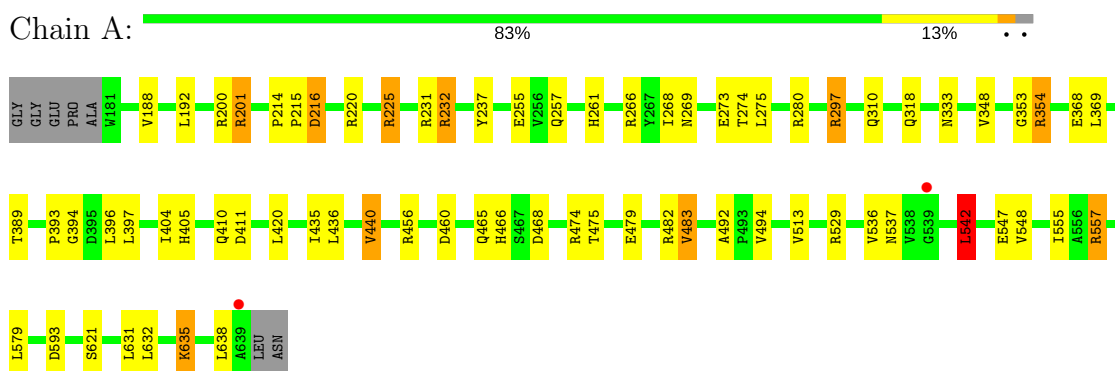
- Molecule 4 is water.

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

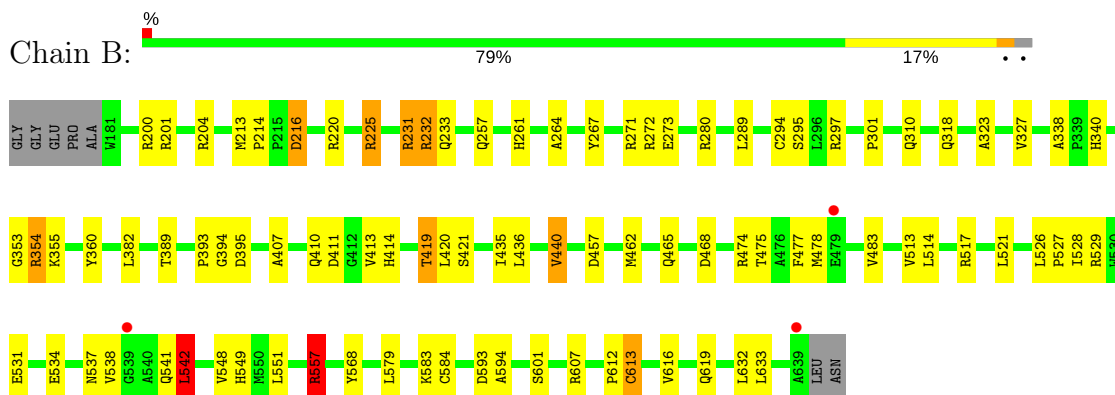
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

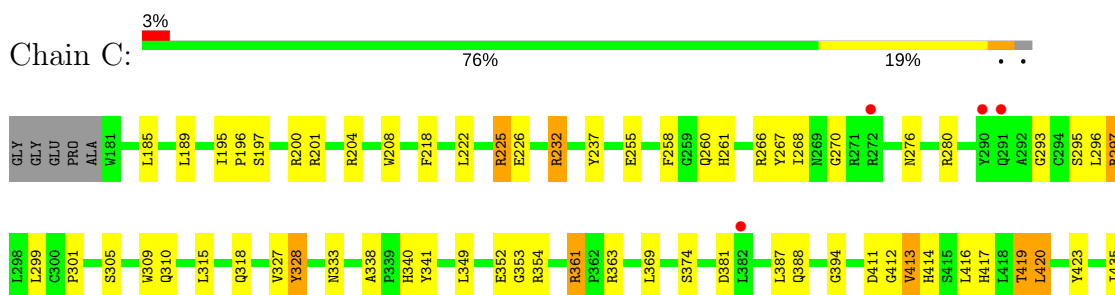
- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66

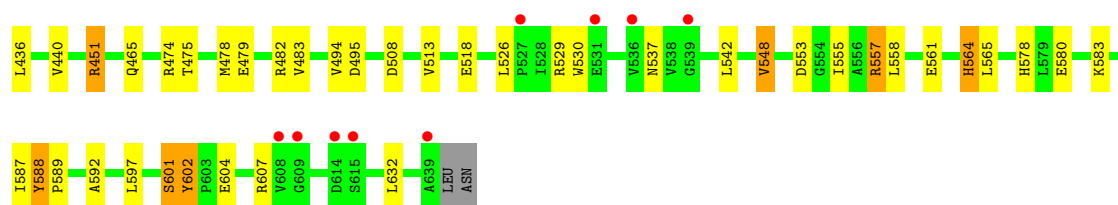


- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66

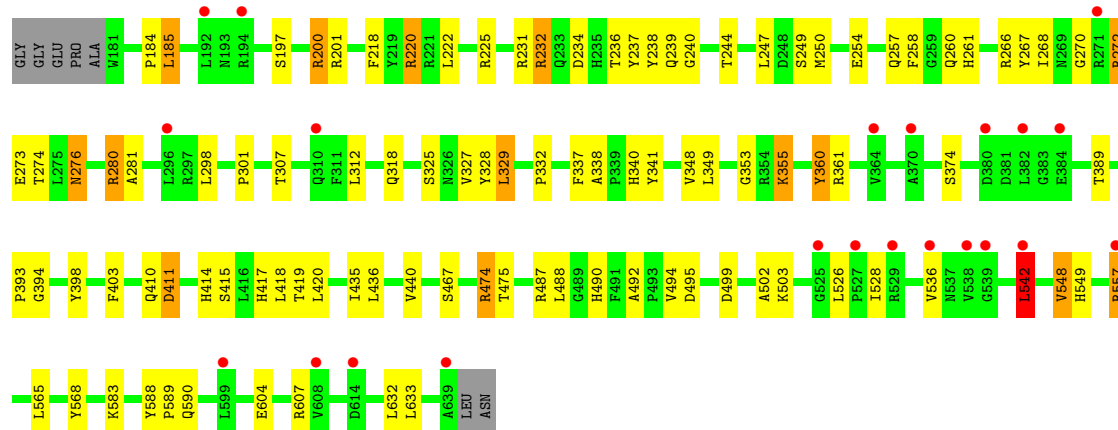
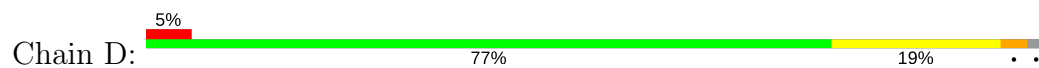


- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.59Å 150.88Å 106.90Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	38.89 – 2.70 38.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.89-2.70) 97.4 (38.86-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.233 , 0.274 0.235 , 0.272	Depositor DCC
$R_{free}$ test set	3556 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , -3.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	14695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.333 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	0.79	0/3755	0.91	9/5113 (0.2%)
1	B	0.77	0/3755	0.92	13/5113 (0.3%)
1	C	0.68	0/3755	0.85	6/5113 (0.1%)
1	D	0.67	0/3771	0.88	9/5133 (0.2%)
All	All	0.73	0/15036	0.89	37/20472 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	B	557	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	D	234	ASP	CB-CA-C	8.09	126.58	110.40
1	C	413	VAL	N-CA-CB	7.70	128.44	111.50
1	D	260	GLN	N-CA-C	-7.40	91.02	111.00
1	A	201	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	225	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	557	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	354	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	613	CYS	N-CA-CB	6.58	122.44	110.60
1	C	412	GLY	N-CA-C	6.49	129.33	113.10
1	C	451	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	260	GLN	N-CA-CB	6.27	121.89	110.60
1	B	201	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	225	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	D	474	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	280	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	234	ASP	N-CA-C	-5.96	94.90	111.00
1	B	395	ASP	CB-CG-OD1	5.92	123.62	118.30
1	B	272	ARG	NE-CZ-NH1	5.83	123.22	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	411	ASP	CB-CA-C	-5.71	98.99	110.40
1	C	474	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	297	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	557	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	231	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	478	MET	CB-CA-C	-5.50	99.40	110.40
1	D	201	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	225	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	225	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	542	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	440	VAL	CB-CA-C	-5.21	101.50	111.40
1	A	440	VAL	CB-CA-C	-5.21	101.51	111.40
1	A	542	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	542	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	204	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	204	ARG	NE-CZ-NH1	5.06	122.83	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	3660	0	3556	49	0
1	B	3660	0	3556	57	0
1	C	3660	0	3556	68	0
1	D	3676	0	3576	68	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14695	0	14253	223	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 (223) 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:B:462:MET:HE2	1:B:477:PHE:CD2	2.04	0.92
1:D:254:GLU:O	1:D:280:ARG:NH2	2.04	0.91
1:B:462:MET:HE2	1:B:477:PHE:CG	2.14	0.82
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: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: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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:312:LEU:HD11	1:D:325:SER:OG	2.04	0.57
1:C:341:TYR:CE2	1:C:374:SER:HB3	2.39	0.57
1:A:354:ARG:HG3	1:A:354:ARG:HH11	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:C:226:GLU:HA	1:C:226:GLU:OE1	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:A:274:THR:C	1:A:275:LEU:HD12	2.26	0.55
1:D:329:LEU:C	1:D:329:LEU:HD12	2.27	0.55
1:B:542:LEU:HD23	1:B:542:LEU:N	2.17	0.55
1:B:557:ARG:HG2	1:B:557:ARG:HH11	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: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:HG21	1:B:632:LEU:HD21	1.89	0.52
1:B:548:VAL:CG2	1:B:632:LEU:CG	2.87	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:548:VAL:HG21	1:D:632:LEU:HD11	1.93	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:H	1:D:542:LEU:HD23	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: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:CD2	1:D:360:TYR:N	2.81	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:HH11	1:C:557:ARG:HG3	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:240:GLY:O	1:D:307:THR:HG21	2.17	0.45
1:B:436:LEU:HD12	1:D:440:VAL:HG22	1.98	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: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: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:B:440:VAL:CG2	1:D:436:LEU:HD12	2.47	0.45
1:C:363:ARG:HH12	1:C:381:ASP:HB3	1.82	0.45
1:B:568:TYR:CD1	1:B:584:CYS:HB3	2.52	0.45
1:C:267:TYR:CE1	1:C:338:ALA:HB2	2.52	0.45
1:C:266:ARG:HD2	1:C:268:ILE:HD11	1.99	0.45
1:A:474:ARG:HH22	1:C:495:ASP:CG	2.20	0.44
1:A:536:VAL:HG23	1:A:537:ASN:ND2	2.32	0.44
1:C:352:GLU:HB2	1:C:416:LEU:HB3	1.98	0.44
1:B:436:LEU:HA	1:B:436:LEU:HD23	1.79	0.44
1:D:398:TYR:C	1:D:398:TYR:CD2	2.90	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:558:LEU:HD11	1:C:587:ILE:HG13	2.00	0.44
1:C:553:ASP:HB2	1:C:602:TYR:CE1	2.53	0.44
1:B:289:LEU:O	1:B:294:CYS:HB2	2.18	0.44
1:C:185:LEU:HD11	1:C:189:LEU:HD11	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:258:PHE:HB3	1:C:276:ASN:HB3	1.99	0.43
1:C:588:TYR:CD1	1:C:588:TYR:N	2.87	0.43
1:B:353:GLY:O	1:B:393:PRO:HD3	2.18	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: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: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:D:220:ARG:HG2	1:D:220:ARG:O	2.19	0.42
1:A:404:ILE:HG22	1:A:405:HIS:N	2.33	0.42
1:D:185:LEU:HD23	1:D:238:TYR:C	2.40	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:A:310:GLN:HA	1:A:513:VAL:HG21	2.02	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:D:185:LEU:CD2	1:D:238:TYR:C	2.88	0.42
1:B:633:LEU:O	1:B:633:LEU:HD12	2.20	0.41
1:C:589:PRO:HA	1:C:592:ALA:HB2	2.02	0.41
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:B:633:LEU:HD12	1:B:633:LEU:C	2.39	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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:201:ARG:NH2	1:C:518:GLU:OE2	2.46	0.41
1:D:267:TYR:CZ	1:D:270:GLY:HA2	2.56	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:C:548:VAL:HG21	1:C:632:LEU:HD11	2.02	0.41
1:A:440:VAL:HG21	1:C:436:LEU:CD1	2.51	0.41
1:D:185:LEU:HD23	1:D:239:GLN:C	2.41	0.41
1:D:418:LEU:C	1:D:418:LEU:HD23	2.42	0.41
1:C:297:ARG:HD3	1:C:328:TYR:CE1	2.56	0.40
1:C:588:TYR:HD1	1:C:588:TYR:N	2.19	0.40
1:B:457:ASP:N	1:B:457:ASP:OD1	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:267:TYR:CE1	1:B:338:ALA:HB2	2.56	0.40
1:B:232:ARG:CD	1:B:394:GLY:O	2.69	0.40
1:C:309:TRP:CD1	1:C:309:TRP:O	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 [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	457/466 (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%)	365 (95%)	21 (5%)	26	54
1	B	386/397 (97%)	356 (92%)	30 (8%)	15	33
1	C	386/397 (97%)	355 (92%)	31 (8%)	14	32
1	D	387/397 (98%)	357 (92%)	30 (8%)	15	33
All	All	1545/1588 (97%)	1433 (93%)	112 (7%)	17	39

All (112) residues with a non-rotameric sidechain are listed below:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	468	ASP
1	A	475	THR
1	A	483	VAL
1	A	542	LEU
1	A	557	ARG
1	A	593	ASP
1	A	621	SER
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	271	ARG
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	465	GLN
1	B	468	ASP
1	B	475	THR
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	583	LYS
1	B	593	ASP
1	B	601	SER
1	B	607	ARG
1	C	197	SER
1	C	200	ARG
1	C	225	ARG
1	C	232	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	255	GLU
1	C	280	ARG
1	C	297	ARG
1	C	305	SER
1	C	318	GLN
1	C	328	TYR
1	C	354	ARG
1	C	361	ARG
1	C	413	VAL
1	C	419	THR
1	C	420	LEU
1	C	465	GLN
1	C	475	THR
1	C	526	LEU
1	C	542	LEU
1	C	548	VAL
1	C	555	ILE
1	C	557	ARG
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	355[A]	LYS
1	D	355[B]	LYS
1	D	360	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	361	ARG
1	D	410	GLN
1	D	411	ASP
1	D	419	THR
1	D	420	LEU
1	D	475	THR
1	D	526	LEU
1	D	542	LEU
1	D	548	VAL
1	D	557	ARG
1	D	565	LEU
1	D	583	LYS
1	D	590	GLN
1	D	604	GLU
1	D	607	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	326	ASN
1	A	333	ASN
1	A	410	GLN
1	A	414	HIS
1	A	466	HIS
1	A	537	ASN
1	A	590	GLN
1	B	261	HIS
1	B	333	ASN
1	B	340	HIS
1	B	414	HIS
1	B	537	ASN
1	B	590	GLN
1	C	261	HIS
1	C	326	ASN
1	C	333	ASN
1	C	340	HIS
1	C	410	GLN
1	C	417	HIS
1	D	261	HIS
1	D	326	ASN
1	D	333	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	340	HIS
1	D	537	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	A	702	2	3,9,9	0.49	0	3,11,11	3.28	1 (33%)
3	OGA	B	702	2	3,9,9	0.78	0	3,11,11	3.55	1 (33%)
3	OGA	C	702	2	3,9,9	0.64	0	3,11,11	3.89	1 (33%)

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	A	702	2	-	0/3/9/9	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OGA	B	702	2	-	0/3/9/9	0/0/0/0
3	OGA	C	702	2	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	OGA	C1-C2-N1	5.35	120.55	115.80
3	B	702	OGA	C1-C2-N1	6.00	121.12	115.80
3	C	702	OGA	C1-C2-N1	6.50	121.57	115.80

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	B	702	OGA	1	0
3	C	702	OGA	2	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 ⓘ

### 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	459/466 (98%)	-0.19	2 (0%) 92 93	11, 25, 49, 76	1 (0%)
1	B	459/466 (98%)	-0.21	3 (0%) 87 88	12, 26, 52, 68	1 (0%)
1	C	459/466 (98%)	0.17	13 (2%) 53 54	13, 44, 76, 103	1 (0%)
1	D	459/466 (98%)	0.30	22 (4%) 31 29	14, 50, 79, 107	1 (0%)
All	All	1836/1864 (98%)	0.02	40 (2%) 62 63	11, 36, 70, 107	4 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	538	VAL	4.4
1	D	639	ALA	4.3
1	B	639	ALA	4.3
1	D	542	LEU	4.0
1	C	539	GLY	3.8
1	C	536	VAL	3.6
1	C	614	ASP	3.6
1	D	527	PRO	3.5
1	C	527	PRO	3.5
1	D	536	VAL	3.4
1	D	382	LEU	3.2
1	C	609	GLY	3.2
1	C	608	VAL	3.2
1	A	539	GLY	3.1
1	D	539	GLY	3.0
1	D	380	ASP	2.8
1	D	384	GLU	2.8
1	C	382	LEU	2.7
1	D	529	ARG	2.5
1	D	296	LEU	2.3
1	D	370	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	608	VAL	2.3
1	C	639	ALA	2.3
1	A	639	ALA	2.3
1	B	539	GLY	2.3
1	D	557	ARG	2.3
1	D	271	ARG	2.2
1	D	525	GLY	2.2
1	C	531	GLU	2.2
1	C	272	ARG	2.2
1	D	614	ASP	2.1
1	C	291	GLN	2.1
1	D	194	ARG	2.1
1	D	599	LEU	2.1
1	B	479	GLU	2.1
1	D	310	GLN	2.1
1	D	192	LEU	2.0
1	D	364	VAL	2.0
1	C	290	TYR	2.0
1	C	615	SER	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	OGA	C	702	10/10	0.86	0.45	5.16	43,53,77,86	0
3	OGA	B	702	10/10	0.95	0.19	1.44	26,27,40,44	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OGA	A	702	10/10	0.97	0.16	0.28	23,24,32,36	0
2	NI	B	701	1/1	0.97	0.07	-	58,58,58,58	0
2	NI	C	701	1/1	0.90	0.11	-	74,74,74,74	0
2	NI	A	701	1/1	0.96	0.04	-	61,61,61,61	0
2	NI	D	701	1/1	0.93	0.05	-	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.