



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:10 am BST

PDB ID : 4CCN  
Title : 60S ribosomal protein L8 histidine hydroxylase (NO66 L299C/C300S) in complex with Mn(II), N-oxalylglycine (NOG) and 60S ribosomal protein L8 (RPL8 G220C) peptide fragment (complex-2)  
Authors : Chowdhury, R.; Schofield, C.J.  
Deposited on : 2013-10-23  
Resolution : 2.23 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

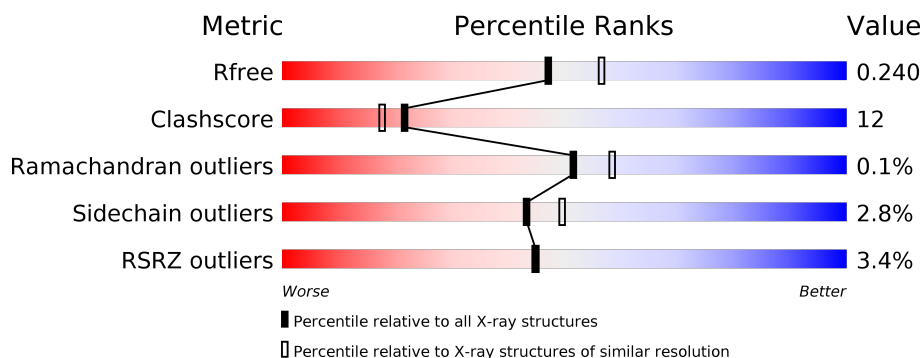
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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))
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 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	467	<div> <div>3%</div> <div>75%</div> <div>23%</div> <div>•</div> </div>
1	B	467	<div> <div>3%</div> <div>72%</div> <div>24%</div> <div>• •</div> </div>
2	C	35	<div> <div>3%</div> <div>20%</div> <div>6%</div> <div>•</div> <div>71%</div> </div>
2	D	35	<div> <div>6%</div> <div>9%</div> <div>20%</div> <div>71%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7936 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	458	Total	C	N	O	S	0	8	0
			3681	2343	657	666	15			
1	B	459	Total	C	N	O	S	0	10	0
			3711	2362	664	670	15			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	expression tag	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
A	299	CYS	LEU	engineered mutation	UNP Q9H6W3
A	300	SER	CYS	engineered mutation	UNP Q9H6W3
A	364	ALA	VAL	engineered mutation	UNP Q9H6W3
B	182	MET	-	expression tag	UNP Q9H6W3
B	642	ALA	-	expression tag	UNP Q9H6W3
B	643	GLU	-	expression tag	UNP Q9H6W3
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
B	299	CYS	LEU	engineered mutation	UNP Q9H6W3
B	300	SER	CYS	engineered mutation	UNP Q9H6W3
B	364	ALA	VAL	engineered mutation	UNP Q9H6W3

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	S	0	0	0
			71	42	16	12	1			
2	D	10	Total	C	N	O	S	0	1	0
			74	44	16	12	2			

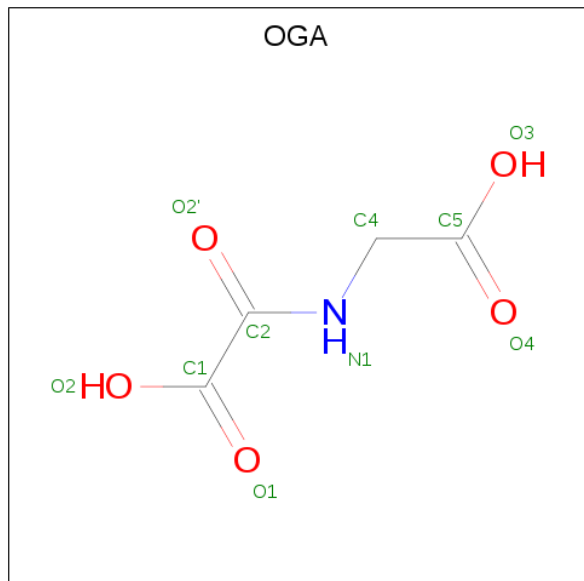
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	220	CYS	GLY	engineered mutation	UNP P62917
D	220	CYS	GLY	engineered mutation	UNP P62917

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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



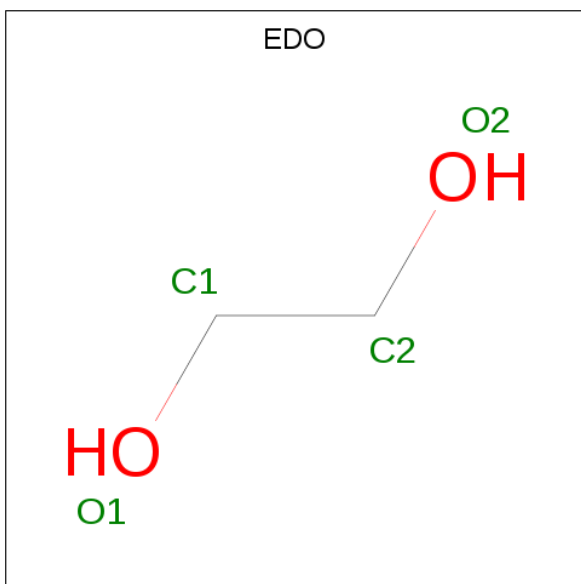
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	4	1	5		
4	B	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

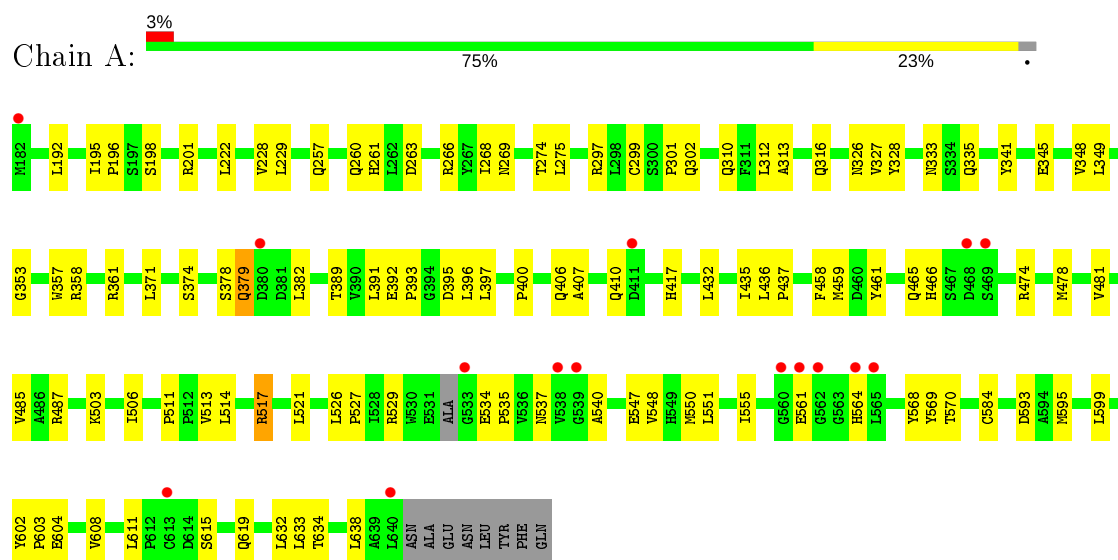
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	192	Total 192	O 192	0	0
7	B	169	Total 169	O 169	0	0
7	C	1	Total 1	O 1	0	0
7	D	1	Total 1	O 1	0	0

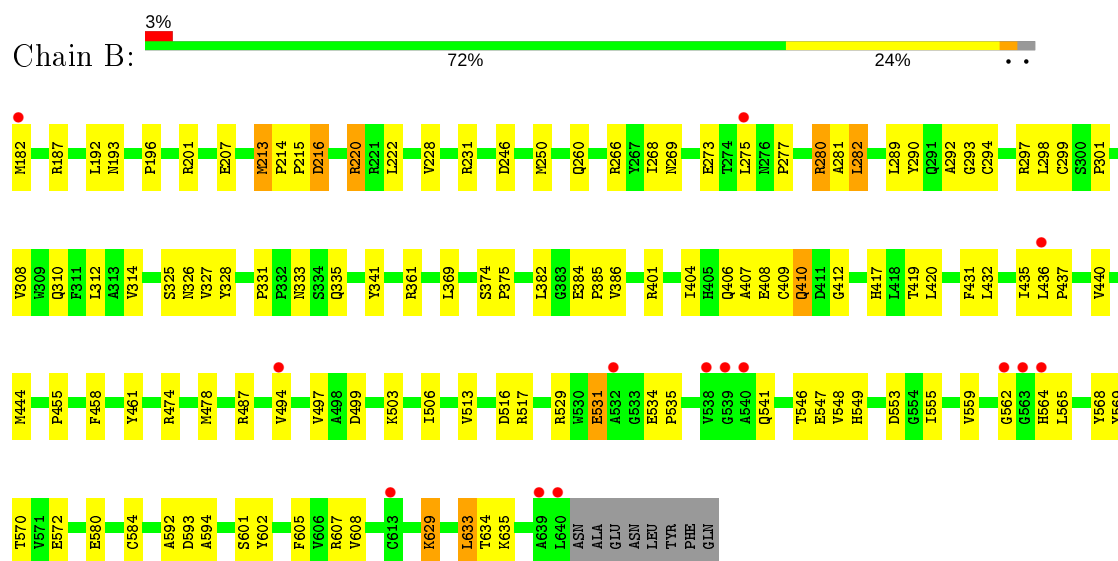
### 3 Residue-property plots [i](#)

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 2: 60S RIBOSOMAL PROTEIN L8





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.16Å 83.72Å 97.03Å 90.00° 100.35° 90.00°	Depositor
Resolution (Å)	44.19 – 2.23 44.19 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.19-2.23) 98.2 (44.19-2.23)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.22Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.238 , 0.248 0.232 , 0.240	Depositor DCC
$R_{free}$ test set	2956 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7936	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 14.65% 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: MN, OGA, SO4, EDO

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	0.41	0/3799	0.63	0/5168
1	B	0.40	0/3836	0.62	0/5219
2	C	0.25	0/73	1.09	1/98 (1.0%)
2	D	0.57	0/79	1.03	1/106 (0.9%)
All	All	0.41	0/7787	0.64	2/10591 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	215	ASN	CB-CA-C	8.52	127.43	110.40
2	C	215	ASN	CB-CA-C	8.48	127.35	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260[A]	GLN	Mainchain
1	A	260[B]	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	379[A]	GLN	Mainchain
1	A	379[B]	GLN	Mainchain
1	A	487[A]	ARG	Mainchain
1	A	487[B]	ARG	Mainchain
1	B	487[A]	ARG	Mainchain
1	B	487[B]	ARG	Mainchain

## 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	3681	0	3597	71	0
1	B	3711	0	3644	103	0
2	C	71	0	57	2	0
2	D	74	0	62	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	3	0	0
4	B	10	0	3	1	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
6	B	4	0	6	2	0
7	A	192	0	0	6	0
7	B	169	0	0	6	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	7936	0	7372	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (178) 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:B:333:ASN:HD21	1:B:412:GLY:H	1.21	0.86
1:B:266[B]:ARG:NH2	1:B:294:CYS:SG	2.51	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280[B]:ARG:HG2	1:B:282:LEU:HD13	1.60	0.83
1:A:268:ILE:HG22	1:A:269[B]:ASN:ND2	2.00	0.76
1:B:266[A]:ARG:HD2	1:B:268:ILE:HD11	1.64	0.76
1:A:229:LEU:HD22	1:A:389:THR:HG21	1.67	0.76
1:B:326:ASN:HD21	2:D:217:GLN:H	1.33	0.74
1:A:432:LEU:HA	1:A:435:ILE:HG22	1.69	0.72
1:B:266[B]:ARG:HB3	1:B:273:GLU:CG	2.20	0.71
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.27	0.69
1:B:280[B]:ARG:HG2	1:B:282:LEU:CD1	2.22	0.69
1:A:335:GLN:HG3	1:A:407:ALA:O	1.92	0.69
1:B:266[A]:ARG:HD2	1:B:268:ILE:CD1	2.22	0.68
1:A:257:GLN:H	1:A:261:HIS:CD2	2.11	0.68
1:B:326:ASN:ND2	2:D:217:GLN:H	1.92	0.68
1:B:266[A]:ARG:HB3	1:B:273:GLU:HG3	1.76	0.68
1:B:266[B]:ARG:HB3	1:B:273:GLU:HG3	1.75	0.68
1:B:326:ASN:HB2	2:D:216:HIS:CE1	2.32	0.65
1:A:257:GLN:H	1:A:261:HIS:HD2	1.44	0.65
1:B:436:LEU:HB2	1:B:437:PRO:HD3	1.79	0.65
1:B:266[B]:ARG:HH12	1:B:293:GLY:HA3	1.63	0.62
1:A:310:GLN:HA	1:A:513:VAL:HG11	1.81	0.61
1:B:266[A]:ARG:HB3	1:B:273:GLU:CG	2.30	0.61
1:B:474:ARG:O	1:B:478:MET:HG2	1.99	0.61
1:B:633:LEU:HD12	1:B:633:LEU:C	2.19	0.61
1:B:222:LEU:HD13	1:B:228:VAL:HG21	1.82	0.61
1:A:503:LYS:HE2	1:A:561:GLU:OE2	2.01	0.60
1:B:297:ARG:HD3	1:B:328:TYR:CE2	2.36	0.60
1:B:266[B]:ARG:HD3	1:B:268:ILE:CD1	2.31	0.60
1:A:268:ILE:HG22	1:A:269[B]:ASN:HD22	1.66	0.60
1:B:266[A]:ARG:HH21	1:B:275:LEU:HD21	1.67	0.59
1:A:548:VAL:HG12	1:A:634:THR:HG22	1.83	0.59
1:A:222:LEU:HD13	1:A:228:VAL:HG21	1.86	0.58
1:B:280[A]:ARG:HG2	1:B:282:LEU:HD13	1.85	0.58
1:B:408:GLU:HG2	6:B:904:EDO:H22	1.87	0.56
1:B:333:ASN:ND2	1:B:412:GLY:H	1.96	0.56
1:B:506:ILE:HG23	1:B:570:THR:CG2	2.35	0.56
1:B:266[B]:ARG:HD3	1:B:268:ILE:HD11	1.87	0.56
1:A:333:ASN:HD22	1:A:410:GLN:HA	1.71	0.55
1:B:503:LYS:HD2	1:B:568:TYR:CZ	2.41	0.55
1:B:572:GLU:OE2	1:B:629:LYS:HE3	2.07	0.55
1:B:222:LEU:HD13	1:B:228:VAL:CG2	2.37	0.55
1:B:280[A]:ARG:HG2	1:B:282:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:TYR:CE1	1:A:603:PRO:HB3	2.44	0.53
1:A:353:GLY:O	1:A:393:PRO:HD3	2.08	0.52
1:B:529[B]:ARG:CZ	1:B:531:GLU:HG2	2.39	0.52
2:D:219:ILE:HG13	2:D:219:ILE:O	2.08	0.52
1:B:406:GLN:HG3	6:B:904:EDO:H12	1.90	0.52
1:B:312:LEU:CD2	1:B:420:LEU:HD13	2.40	0.52
1:A:547:GLU:OE2	5:A:903:SO4:O2	2.26	0.52
1:A:222:LEU:HD13	1:A:228:VAL:CG2	2.40	0.52
1:A:465:GLN:HE21	1:A:466:HIS:CE1	2.28	0.52
1:B:266[B]:ARG:HH22	1:B:292:ALA:C	2.14	0.51
1:B:335:GLN:HG3	1:B:407:ALA:O	2.10	0.51
1:A:313:ALA:O	1:A:316:GLN:HG2	2.09	0.51
1:B:216:ASP:OD1	1:B:220:ARG:NH1	2.44	0.51
1:B:513:VAL:HG23	1:B:513:VAL:O	2.11	0.51
1:B:207[B]:GLU:HG2	1:B:215:PRO:HG2	1.92	0.51
1:B:435:ILE:HD13	1:B:497:VAL:HG21	1.93	0.51
1:A:299:CYS:HA	1:A:326:ASN:ND2	2.25	0.50
1:A:459:MET:HE2	7:A:2134:HOH:O	2.12	0.50
1:B:601:SER:HB2	7:B:2162:HOH:O	2.12	0.50
1:A:529:ARG:HH12	1:A:537:ASN:HD22	1.57	0.50
1:A:302:GLN:HB3	1:A:312:LEU:HD12	1.93	0.49
1:A:633:LEU:C	1:A:633:LEU:HD12	2.32	0.49
1:A:511:PRO:HB2	7:A:2149:HOH:O	2.11	0.49
1:B:341:TYR:CE2	1:B:374:SER:HB3	2.48	0.49
1:A:432:LEU:HA	1:A:435:ILE:CG2	2.39	0.49
1:B:506:ILE:HG23	1:B:570:THR:HG22	1.95	0.48
1:A:345:GLU:OE1	1:A:400:PRO:HA	2.14	0.48
1:B:231:ARG:HG3	7:B:2031:HOH:O	2.12	0.48
1:B:310:GLN:O	1:B:314:VAL:HG23	2.13	0.48
1:B:409:CYS:C	1:B:410:GLN:HG3	2.34	0.48
1:B:541:GLN:HA	7:B:2142:HOH:O	2.13	0.48
1:A:371:LEU:HD11	1:B:444:MET:HB3	1.95	0.48
1:A:506:ILE:O	1:A:570:THR:HG22	2.14	0.48
1:B:546:THR:O	1:B:608:VAL:HG23	2.14	0.48
1:B:529[B]:ARG:NH1	1:B:531:GLU:OE2	2.46	0.47
1:A:481:VAL:O	1:A:485:VAL:HG23	2.14	0.47
1:B:192:LEU:O	1:B:201:ARG:HD2	2.14	0.47
1:B:275:LEU:N	1:B:275:LEU:HD12	2.29	0.47
1:B:529[A]:ARG:NH2	1:B:531:GLU:OE2	2.47	0.47
1:A:435:ILE:HG23	1:A:436:LEU:N	2.30	0.47
1:A:608:VAL:O	1:A:611:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ILE:O	1:A:569:TYR:HA	2.15	0.47
1:A:432:LEU:CA	1:A:435:ILE:HG22	2.43	0.47
1:B:266[B]:ARG:HB3	1:B:273:GLU:HG2	1.97	0.47
1:A:540:ALA:HB1	1:A:638:LEU:HB3	1.97	0.47
1:B:374:SER:HB2	1:B:375:PRO:HD2	1.97	0.47
1:B:548:VAL:HG12	1:B:634:THR:HG22	1.96	0.47
1:B:534:GLU:HB2	1:B:535:PRO:HD2	1.97	0.47
1:B:301:PRO:HG2	1:B:308:VAL:HG11	1.97	0.46
7:B:2118:HOH:O	2:D:219:ILE:HG12	2.15	0.46
1:B:250:MET:CE	1:B:298:LEU:HD21	2.45	0.46
1:B:417:HIS:HE1	4:B:902:OGA:O1	1.98	0.46
1:A:275:LEU:HD12	1:A:275:LEU:N	2.30	0.46
1:B:266[B]:ARG:NH2	1:B:292:ALA:O	2.49	0.46
1:B:506:ILE:HG23	1:B:570:THR:HG23	1.97	0.46
1:A:432:LEU:O	1:A:435:ILE:HG22	2.16	0.45
1:B:437:PRO:O	1:B:440:VAL:HG12	2.16	0.45
1:B:182:MET:HG3	1:B:187:ARG:HG2	1.98	0.45
1:B:455:PRO:HB2	1:B:458:PHE:HB3	1.98	0.45
1:B:553:ASP:HB2	1:B:602:TYR:CD2	2.51	0.45
1:A:550:MET:HE2	1:A:632:LEU:CD1	2.47	0.45
1:B:290:TYR:CD1	1:B:331:PRO:HG3	2.51	0.45
1:B:341:TYR:CE1	1:B:374:SER:HB3	2.51	0.45
1:B:299:CYS:SG	2:D:220[B]:CYS:HB3	2.56	0.45
1:A:474:ARG:O	1:A:478:MET:HG2	2.17	0.44
1:B:193[B]:ASN:ND2	1:B:516:ASP:OD2	2.39	0.44
1:A:266:ARG:HD3	1:A:268:ILE:HD11	1.99	0.44
1:A:458:PHE:HA	1:A:461:TYR:CZ	2.52	0.44
1:B:547:GLU:HA	1:B:607:ARG:HA	1.98	0.44
1:A:514:LEU:HD21	1:A:551:LEU:HD21	1.98	0.44
1:A:513:VAL:O	1:A:513:VAL:HG23	2.18	0.44
1:B:268:ILE:HG22	1:B:269[A]:ASN:OD1	2.17	0.44
1:B:565:LEU:HD13	1:B:592:ALA:HB2	2.00	0.44
1:A:301:PRO:HG3	1:A:327:VAL:HG23	1.98	0.44
1:A:349:LEU:HD12	1:A:349:LEU:N	2.33	0.44
1:A:192:LEU:HD22	1:A:201:ARG:HG3	2.00	0.43
1:A:550:MET:HE2	1:A:632:LEU:HD12	2.00	0.43
1:B:213:MET:O	1:B:213:MET:HG3	2.18	0.43
1:B:580:GLU:HB2	7:B:2153:HOH:O	2.16	0.43
1:A:274:THR:C	1:A:275:LEU:HD12	2.39	0.43
1:B:301:PRO:HG3	1:B:327:VAL:HG23	2.00	0.43
2:C:215:ASN:HA	2:C:215:ASN:HD22	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LEU:HA	1:B:401:ARG:HG3	2.01	0.43
1:A:349:LEU:O	1:A:417:HIS:HB2	2.19	0.43
1:A:379[B]:GLN:OE1	1:A:406:GLN:NE2	2.41	0.43
1:A:526:LEU:HA	1:A:527:PRO:HD3	1.83	0.43
1:B:275:LEU:O	1:B:277:PRO:HD3	2.18	0.43
1:A:568:TYR:CD1	1:A:584:CYS:HB3	2.54	0.43
1:B:458:PHE:HA	1:B:461:TYR:CE2	2.54	0.43
1:B:529[B]:ARG:NH2	1:B:531:GLU:HG2	2.34	0.42
1:B:593:ASP:OD1	1:B:594:ALA:N	2.51	0.42
1:B:213:MET:HA	1:B:214:PRO:HD3	1.83	0.42
1:B:266[B]:ARG:HD3	1:B:268:ILE:HD12	2.00	0.42
1:B:499:ASP:HB3	1:B:559:VAL:HG13	2.01	0.42
1:A:348:VAL:HB	1:A:397:LEU:HB3	2.00	0.42
1:A:459:MET:HG3	7:A:2134:HOH:O	2.18	0.42
1:A:378:SER:HB3	7:A:2109:HOH:O	2.20	0.42
1:B:182:MET:CG	1:B:187:ARG:HG2	2.49	0.42
1:A:357:TRP:CD1	1:A:391:LEU:HD12	2.55	0.42
1:B:214:PRO:HA	1:B:215:PRO:HD3	1.91	0.42
1:B:431:PHE:CZ	1:B:494:VAL:HG13	2.55	0.42
1:A:266:ARG:HD3	1:A:268:ILE:CD1	2.50	0.42
1:A:297:ARG:HG3	1:A:328:TYR:CE2	2.55	0.42
1:A:361:ARG:HH11	1:A:361:ARG:HB3	1.84	0.42
1:B:568:TYR:CD2	1:B:584:CYS:HB3	2.55	0.42
1:A:595:MET:HE2	1:A:599:LEU:HG	2.01	0.41
1:A:392:GLU:HG2	1:A:395:ASP:OD2	2.20	0.41
1:B:193[A]:ASN:HD21	1:B:516:ASP:H	1.68	0.41
1:B:266[B]:ARG:HD2	1:B:273:GLU:OE2	2.20	0.41
1:A:341:TYR:CZ	1:A:374:SER:HB3	2.56	0.41
1:A:615:SER:O	1:A:619:GLN:HG3	2.21	0.41
1:B:246:ASP:O	1:B:250:MET:HB2	2.20	0.41
1:B:361:ARG:HG3	1:B:386:VAL:HB	2.02	0.41
1:B:555:ILE:O	1:B:569:TYR:HA	2.20	0.41
1:A:195:ILE:HA	1:A:196:PRO:HD3	1.95	0.41
1:A:358:ARG:NH1	7:A:2095:HOH:O	2.48	0.41
2:D:221:LYS:CB	2:D:222:PRO:HD2	2.51	0.41
1:B:605:PHE:CZ	1:B:635:LYS:HA	2.55	0.41
1:A:534:GLU:CG	1:A:535:PRO:HD2	2.51	0.41
1:B:458:PHE:HA	1:B:461:TYR:CZ	2.56	0.41
1:A:436:LEU:HB2	1:A:437:PRO:HD3	2.02	0.40
1:A:529:ARG:NH1	1:A:537:ASN:HD22	2.19	0.40
1:B:325:SER:HA	1:B:419:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LEU:HD22	1:B:404:ILE:HG21	2.03	0.40
1:B:417:HIS:HD2	7:B:2077:HOH:O	2.04	0.40
1:B:562:GLY:O	1:B:564:HIS:HD2	2.04	0.40
7:A:2076:HOH:O	2:C:216:HIS:HB2	2.20	0.40
1:A:198:SER:HB3	1:A:201:ARG:NH2	2.36	0.40
1:A:529:ARG:HH12	1:A:537:ASN:ND2	2.18	0.40
1:B:384:GLU:HA	1:B:385:PRO:HD3	1.93	0.40
1:A:348:VAL:HG13	1:A:417:HIS:CD2	2.56	0.40
1:A:517[B]:ARG:CZ	1:A:521:LEU:HD11	2.51	0.40
1:B:266[B]:ARG:HH12	1:B:293:GLY:CA	2.29	0.40
1:B:280[B]:ARG:HG3	1:B:281:ALA:N	2.37	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	462/467 (99%)	452 (98%)	10 (2%)	0	100	100
1	B	467/467 (100%)	451 (97%)	15 (3%)	1 (0%)	47	53
2	C	8/35 (23%)	6 (75%)	2 (25%)	0	100	100
2	D	9/35 (26%)	8 (89%)	1 (11%)	0	100	100
All	All	946/1004 (94%)	917 (97%)	28 (3%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	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	387/399 (97%)	379 (98%)	8 (2%)	53	60
1	B	392/399 (98%)	377 (96%)	15 (4%)	33	36
2	C	7/27 (26%)	6 (86%)	1 (14%)	3	1
2	D	8/27 (30%)	8 (100%)	0	100	100
All	All	794/852 (93%)	770 (97%)	24 (3%)	43	47

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

Mol	Chain	Res	Type
1	A	263	ASP
1	A	382	LEU
1	A	396	LEU
1	A	517[A]	ARG
1	A	517[B]	ARG
1	A	564	HIS
1	A	593	ASP
1	A	604	GLU
1	B	213	MET
1	B	216	ASP
1	B	220	ARG
1	B	260	GLN
1	B	280[A]	ARG
1	B	280[B]	ARG
1	B	282	LEU
1	B	289	LEU
1	B	410	GLN
1	B	432	LEU
1	B	517	ARG
1	B	531	GLU
1	B	549	HIS
1	B	629	LYS
1	B	633	LEU
2	C	217	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	261	HIS
1	A	333	ASN
1	A	376	ASN
1	A	388	GLN
1	A	410	GLN
1	A	465	GLN
1	A	537	ASN
1	A	619	GLN
1	B	239	GLN
1	B	261	HIS
1	B	326	ASN
1	B	333	ASN
1	B	376	ASN
1	B	379	GLN
1	B	406	GLN
1	B	417	HIS
1	B	441	GLN
1	B	466	HIS
1	B	591	GLN
2	C	215	ASN
2	C	217	GLN
2	D	215	ASN
2	D	217	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z  > 2$
5	SO4	A	903	-	4,4,4	0.31	0	6,6,6	0.12	0
4	OGA	A	902	3	3,9,9	0.46	0	4,11,11	1.51	1 (25%)
4	OGA	B	902	3	3,9,9	0.44	0	4,11,11	1.48	1 (25%)
6	EDO	B	904	-	3,3,3	0.47	0	2,2,2	0.33	0
5	SO4	B	903	-	4,4,4	0.27	0	6,6,6	0.06	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
4	OGA	A	902	3	-	0/3/9/9	-
4	OGA	B	902	3	-	0/3/9/9	-
6	EDO	B	904	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	OGA	C1-C2-N1	2.97	118.55	115.60
4	B	902	OGA	C1-C2-N1	2.92	118.50	115.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	904	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	903	SO4	1	0
4	B	902	OGA	1	0
6	B	904	EDO	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	458/467 (98%)	0.25	15 (3%)	46 46	17, 35, 62, 73	6 (1%)
1	B	459/467 (98%)	0.31	14 (3%)	49 49	16, 35, 66, 77	2 (0%)
2	C	10/35 (28%)	0.85	1 (10%)	7 6	32, 38, 67, 72	2 (20%)
2	D	10/35 (28%)	1.35	2 (20%)	1 1	33, 39, 63, 67	2 (20%)
All	All	937/1004 (93%)	0.30	32 (3%)	45 45	16, 35, 65, 77	12 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	GLY	4.6
2	D	213	GLY	4.0
1	B	639	ALA	4.0
2	D	222	PRO	3.9
1	B	532	ALA	3.7
2	C	222	PRO	3.5
1	A	640	LEU	3.4
1	A	613	CYS	3.4
1	A	533	GLY	3.3
1	B	640	LEU	3.2
1	A	538	VAL	3.2
1	A	561	GLU	3.1
1	B	539	GLY	3.1
1	A	468	ASP	2.9
1	B	538	VAL	2.8
1	A	565	LEU	2.8
1	A	562	GLY	2.8
1	A	564	HIS	2.7
1	B	613	CYS	2.6
1	B	564	HIS	2.6
1	B	275	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	436	LEU	2.5
1	A	539	GLY	2.3
1	A	469	SER	2.3
1	B	540	ALA	2.3
1	A	560	GLY	2.3
1	A	182	MET	2.2
1	A	411	ASP	2.1
1	B	182	MET	2.1
1	A	380	ASP	2.0
1	B	494	VAL	2.0
1	B	563	GLY	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	903	5/5	0.46	0.33	98,100,101,101	5
5	SO4	B	903	5/5	0.78	0.29	102,102,103,103	0
4	OGA	A	902	10/10	0.90	0.15	33,35,42,44	0
6	EDO	B	904	4/4	0.91	0.22	29,31,33,37	0
4	OGA	B	902	10/10	0.94	0.14	22,27,35,35	0
3	MN	B	901	1/1	0.97	0.13	19,19,19,19	0
3	MN	A	901	1/1	0.99	0.13	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.