



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2014 – 06:21 AM EDT

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 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/ValidationPDFNotes.html>

---

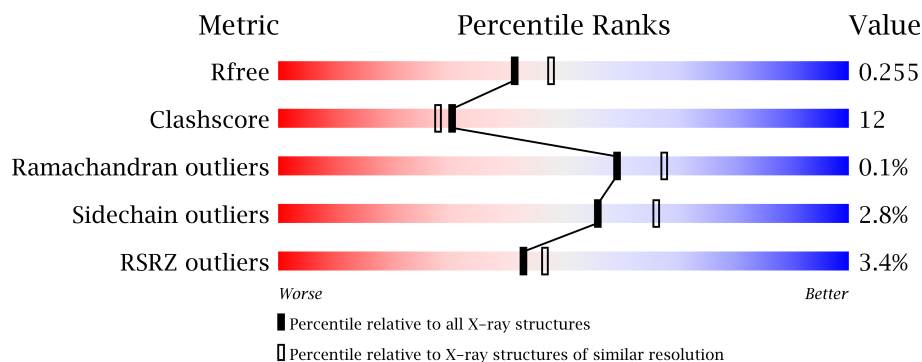
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	467	
1	B	467	
2	C	35	
2	D	35	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	903	-	X
5	SO4	B	903	-	X
6	EDO	B	904	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7936 atoms, of which 0 are hydrogen and 0 are deuterium.

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 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	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	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			

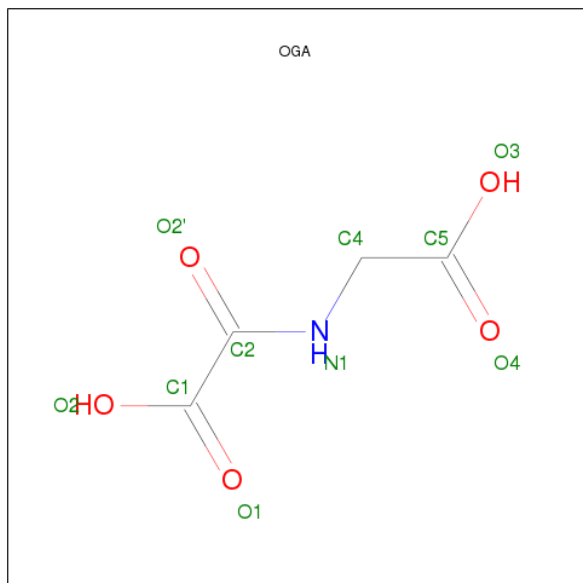
There are 2 discrepancies between the modelled and reference sequences:

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).

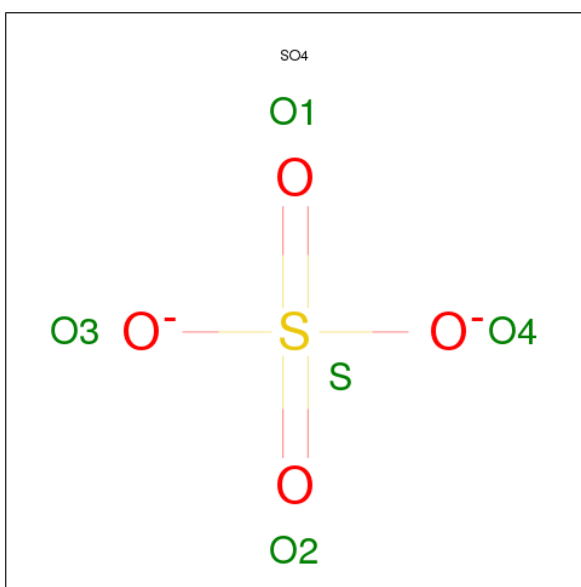
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

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



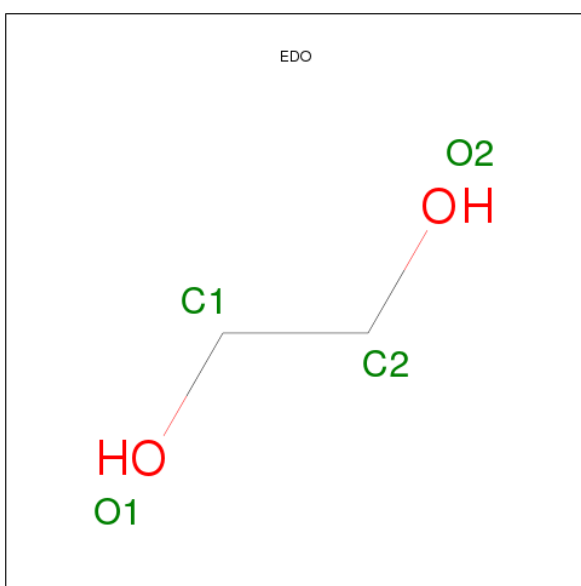
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	4	1	5		
4	B	1	Total	C	N	O	0	0
			10	4	1	5		

- 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:  $C_2H_6O_2$ ).



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

- Molecule 7 is water.

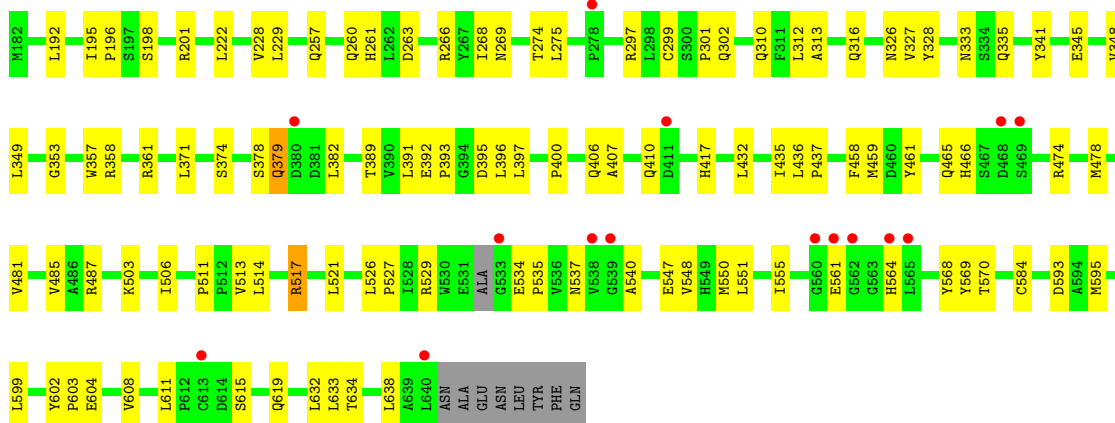
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	192	Total 192	O 192	0	0
7	B	169	Total 169	O 169	0	0
7	C	1	Total 1	O 1	0	0
7	D	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

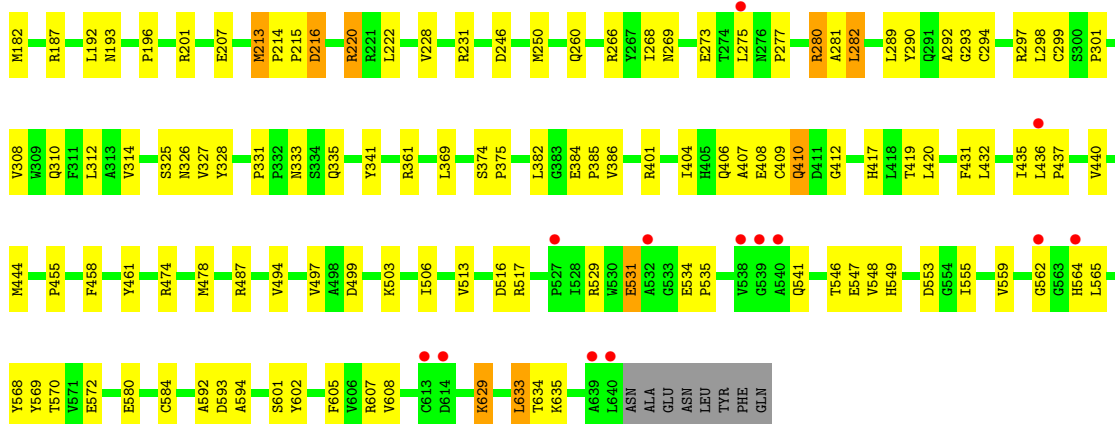
#### • Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

Chain A: 



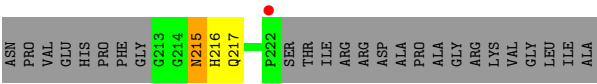
#### • Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

Chain B: 



#### • Molecule 2: 60S RIBOSOMAL PROTEIN L8

Chain C: 



● Molecule 2: 60S RIBOSOMAL PROTEIN L8

Chain D:





## 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 0.248 , 0.255	Depositor DCC
$R_{free}$ test set	2955 reflections (5.04%)	DCC
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> )	0.34 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 58651 reflections (0.002%)	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.

## 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

*Continued on next page...*

*Continued from previous page...*

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(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:333:ASN:ND2	1:B:412:GLY:H	1.96	0.56
1:B:408:GLU:HG2	6:B:904:EDO:H22	1.87	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
1:A:602:TYR:CE1	1:A:603:PRO:HB3	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:369:LEU:HA	1:B:401:ARG:HG3	2.01	0.43
1:A:379[B]:GLN:OE1	1:A:406:GLN:NE2	2.41	0.43
1:A:349:LEU:O	1:A:417:HIS:HB2	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:266[B]:ARG:HD2	1:B:273:GLU:OE2	2.20	0.41
1:B:193[A]:ASN:HD21	1:B:516:ASP:H	1.68	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
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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	56	63
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%)	59	67

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%)	66	76
1	B	392/399 (98%)	377 (96%)	15 (4%)	44	52
2	C	7/27 (26%)	6 (86%)	1 (14%)	5	2
2	D	8/27 (30%)	8 (100%)	0	100	100
All	All	794/852 (93%)	770 (97%)	24 (3%)	56	63

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

### 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

### 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.8 Polymer linkage issues

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%)	0.29	15 (3%) 44 48	17, 35, 62, 73	6 (1%)
1	B	459/467 (98%)	0.33	13 (2%) 50 55	16, 35, 66, 77	2 (0%)
2	C	10/35 (28%)	0.89	1 (10%) 8 9	32, 38, 67, 72	2 (20%)
2	D	10/35 (28%)	1.37	2 (20%) 2 1	33, 39, 63, 67	2 (20%)
All	All	937/1004 (93%)	0.33	31 (3%) 43 48	16, 35, 65, 77	12 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	GLY	4.4
2	D	222	PRO	4.3
1	B	532	ALA	4.1
1	B	640	LEU	4.0
2	C	222	PRO	4.0
2	D	213	GLY	3.9
1	A	640	LEU	3.8
1	B	639	ALA	3.7
1	A	533	GLY	3.6
1	A	561	GLU	3.3
1	A	613	CYS	3.3
1	B	538	VAL	3.2
1	A	560	GLY	2.9
1	B	539	GLY	2.8
1	A	562	GLY	2.7
1	B	613	CYS	2.7
1	A	538	VAL	2.6
1	B	564	HIS	2.6
1	A	564	HIS	2.6
1	B	275	LEU	2.6
1	A	468	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	278	PRO	2.5
1	A	539	GLY	2.5
1	A	411	ASP	2.3
1	B	540	ALA	2.2
1	A	469	SER	2.2
1	A	380	ASP	2.2
1	A	565	LEU	2.2
1	B	614	ASP	2.1
1	B	436	LEU	2.1
1	B	527	PRO	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	903	5/5	0.36	7.84	98,100,101,101	5
5	SO4	B	903	5/5	0.31	3.01	102,102,103,103	0
6	EDO	B	904	4/4	0.23	2.74	29,31,33,37	0
4	OGA	B	902	10/10	0.13	0.23	22,27,35,35	0
4	OGA	A	902	10/10	0.14	-0.09	33,35,42,44	0
3	MN	B	901	1/1	0.12	-1.21	19,19,19,19	0
3	MN	A	901	1/1	0.13	-1.27	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.