



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 07:49 pm GMT

PDB ID : 4CCO  
Title : 60S ribosomal protein L8 histidine hydroxylase (NO66 S373C) in complex with Mn(II), N-oxalylglycine (NOG) and 60S ribosomal protein L8 (RPL8 G214C) peptide fragment (complex-3)  
Authors : Chowdhury, R.; Schofield, C.J.  
Deposited on : 2013-10-23  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

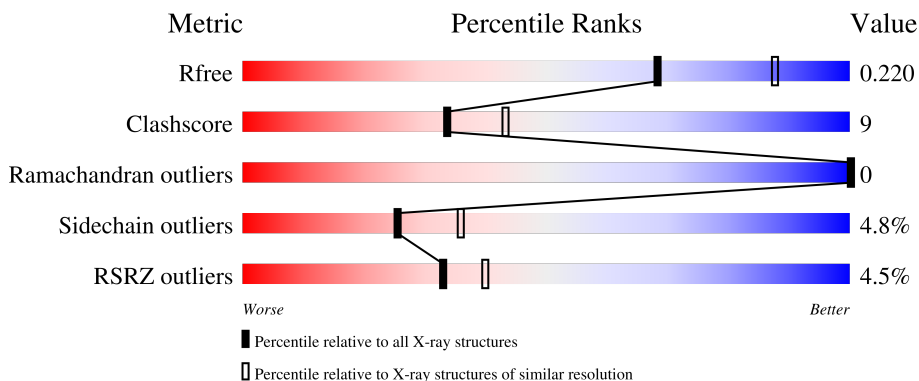
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	 3% 79% 17% ..
1	B	467	 3% 82% 15% ..
2	C	20	 35% 25% 15% 20% 40%
2	D	20	 30% 40% 15% 5% 40%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8128 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
			Total	C	N	O	S			
1	A	458	3689	2346	652	674	17	0	5	0
1	B	459	3687	2346	655	669	17	0	4	0

There are 20 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	364	ALA	VAL	engineered mutation	UNP Q9H6W3
A	373	CYS	SER	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	364	ALA	VAL	engineered mutation	UNP Q9H6W3
B	373	CYS	SER	engineered mutation	UNP Q9H6W3

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			84	50	19	15			
2	D	12	Total	C	N	O	S	0	0
			85	50	19	15	1		

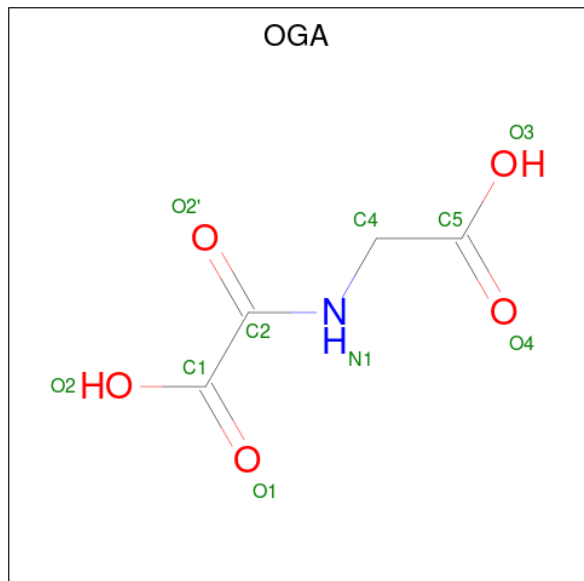
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	214	CYS	GLY	engineered mutation	UNP P62917
D	214	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	A	1	Total	Mn	0	0
			1	1		
3	B	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

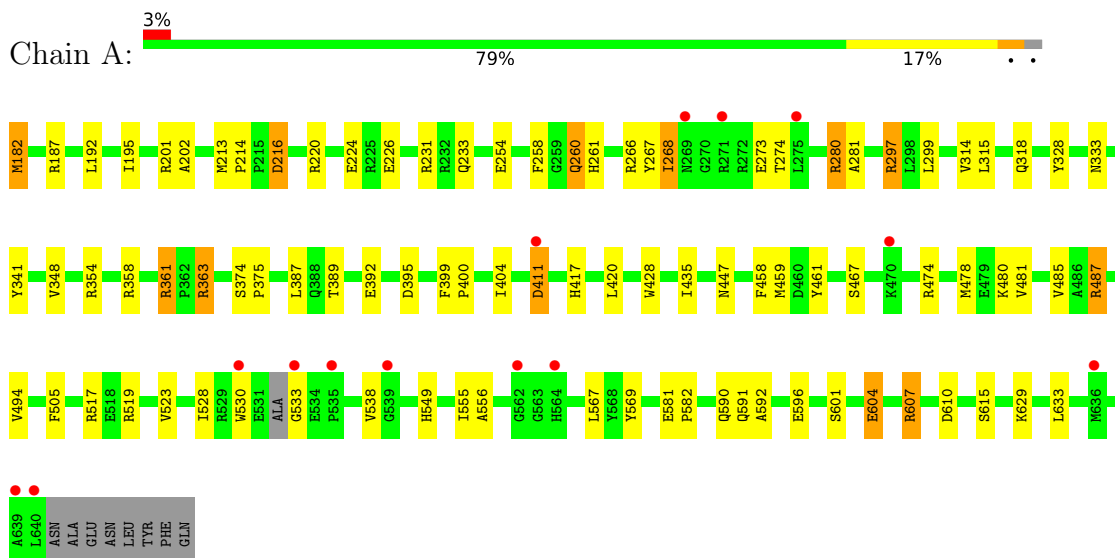
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	287	Total O 287 287	0	0
6	B	253	Total O 253 253	0	0
6	D	1	Total O 1 1	0	0

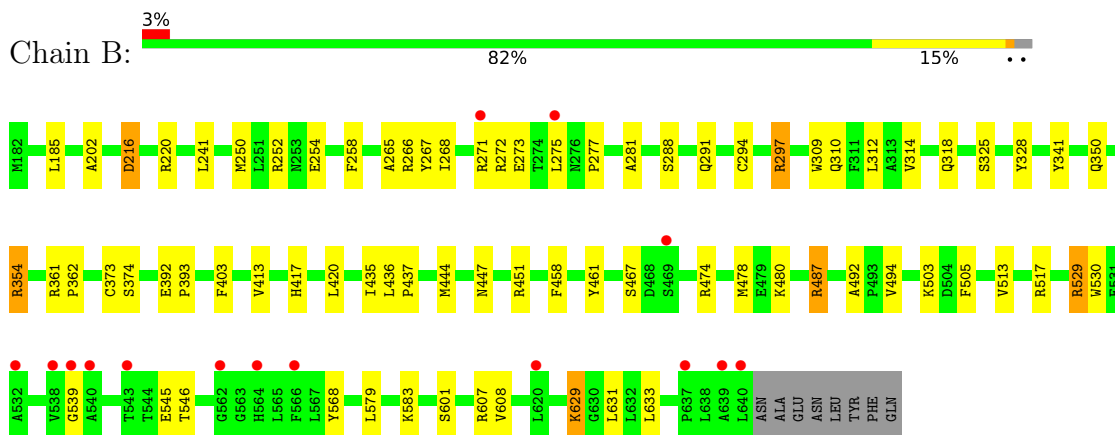
### 3 Residue-property plots

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

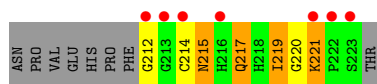


- Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

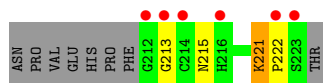


- Molecule 2: 60S RIBOSOMAL PROTEIN L8





- 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, $\alpha$ , $\beta$ , $\gamma$	155.39Å 84.94Å 97.30Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	43.70 – 2.30 43.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (43.70-2.30) 97.9 (43.70-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.210 , 0.225 0.205 , 0.220	Depositor DCC
$R_{free}$ test set	2761 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtrriage
Anisotropy	0.724	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.88% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, OGA, 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	0.40	0/3798	0.67	0/5167
1	B	0.40	0/3794	0.67	1/5163 (0.0%)
2	C	0.39	0/86	0.65	0/114
2	D	0.41	0/87	0.62	0/115
All	All	0.40	0/7765	0.67	1/10559 (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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	539	GLY	N-CA-C	5.15	125.97	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	3689	0	3604	72	0
1	B	3687	0	3609	53	0
2	C	84	0	74	9	0
2	D	85	0	77	3	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	0	0
5	A	8	0	12	2	0
5	B	12	0	18	2	0
6	A	287	0	0	7	0
6	B	253	0	0	4	0
6	D	1	0	0	0	0
All	All	8128	0	7400	128	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 9.

All (128) 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:528:ILE:HD12	1:A:538:VAL:CB	1.63	1.29
1:A:392[B]:GLU:HG2	1:A:395:ASP:OD2	1.48	1.10
1:A:231[B]:ARG:NH2	1:A:392[B]:GLU:HG3	1.67	1.10
1:A:274:THR:HG23	6:A:2075:HOH:O	1.63	0.97
1:B:447:ASN:HD21	1:B:487[A]:ARG:HH12	1.23	0.86
1:A:528:ILE:CD1	1:A:538:VAL:CB	2.53	0.85
1:A:231[B]:ARG:NH2	1:A:392[B]:GLU:CG	2.42	0.82
1:B:447:ASN:HD21	1:B:487[A]:ARG:NH1	1.85	0.74
1:A:231[B]:ARG:CZ	1:A:392[B]:GLU:HG3	2.18	0.74
1:A:274:THR:CG2	6:A:2075:HOH:O	2.25	0.73
1:A:266:ARG:HD3	1:A:268:ILE:HD11	1.71	0.73
1:B:216:ASP:OD2	1:B:220[A]:ARG:NH2	2.24	0.70
1:B:373:CYS:SG	6:B:2133:HOH:O	2.48	0.69
1:B:447:ASN:ND2	1:B:487[A]:ARG:NH1	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ARG:NH1	6:B:2010:HOH:O	2.26	0.67
1:B:275:LEU:HD22	1:B:294:CYS:SG	2.35	0.67
1:A:629:LYS:NZ	6:A:2257:HOH:O	2.28	0.66
1:A:216[B]:ASP:OD1	1:A:220:ARG:NH2	2.30	0.65
1:A:231[B]:ARG:HH21	1:A:392[B]:GLU:CD	2.01	0.62
1:A:231[B]:ARG:HH11	1:A:233:GLN:H	1.47	0.61
1:A:467:SER:HA	1:A:474:ARG:NH2	2.16	0.60
1:B:529:ARG:HG2	1:B:530:TRP:N	2.17	0.60
1:B:373:CYS:HB2	2:D:213:GLY:O	2.01	0.59
1:B:297:ARG:NH1	2:D:215:ASN:O	2.35	0.59
1:A:315:LEU:HD12	1:A:420:LEU:HD11	1.84	0.58
1:A:363:ARG:HD3	1:A:404:ILE:HD12	1.85	0.58
1:A:363:ARG:HD3	1:A:404:ILE:CD1	2.34	0.58
2:C:214:CYS:O	2:C:217:GLN:NE2	2.37	0.58
1:A:231[A]:ARG:NH2	1:A:389:THR:OG1	2.37	0.57
1:A:517:ARG:NH2	6:A:2236:HOH:O	2.31	0.56
1:A:297:ARG:NH1	2:C:215:ASN:O	2.37	0.55
1:B:436:LEU:HB2	1:B:437:PRO:HD3	1.88	0.55
1:A:428:TRP:CZ2	1:B:480:LYS:HD3	2.42	0.54
1:B:505:PHE:HB2	5:B:904:EDO:H11	1.89	0.54
1:A:258:PHE:CE2	1:A:281:ALA:HA	2.44	0.53
1:B:354[A]:ARG:HD2	6:B:2104:HOH:O	2.07	0.53
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.44	0.52
1:A:267:TYR:C	1:A:268:ILE:HG12	2.30	0.52
1:A:297:ARG:HD2	1:A:299:LEU:HD23	1.93	0.51
1:A:530:TRP:CZ2	1:A:533:GLY:HA2	2.45	0.51
1:A:231[B]:ARG:NH2	1:A:392[B]:GLU:CD	2.63	0.51
2:C:219:ILE:HD12	2:C:221:LYS:HG2	1.93	0.51
1:A:231[B]:ARG:NH1	1:A:233:GLN:HA	2.26	0.51
1:A:260:GLN:HG2	1:A:261:HIS:CE1	2.46	0.50
1:B:629:LYS:HB3	1:B:631:LEU:HG	1.92	0.50
2:C:217:GLN:HE21	2:C:217:GLN:HA	1.76	0.50
1:B:545:GLU:OE2	1:B:607:ARG:NH1	2.46	0.49
1:A:480:LYS:NZ	6:A:2192:HOH:O	2.45	0.49
1:B:546:THR:O	1:B:608:VAL:HG23	2.12	0.49
1:B:297:ARG:HG3	1:B:328:TYR:CE2	2.48	0.49
1:A:375:PRO:HA	2:C:212:GLY:HA3	1.95	0.48
1:A:254:GLU:O	1:A:280:ARG:NH2	2.45	0.48
1:A:226:GLU:OE2	1:A:361:ARG:NH2	2.47	0.48
1:A:192:LEU:HA	1:A:195:ILE:HD12	1.96	0.48
1:B:220[A]:ARG:NH1	6:B:2030:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:OD1	1:A:411:ASP:HA	2.14	0.47
1:B:341:TYR:CE1	1:B:374:SER:HB3	2.49	0.47
1:A:435:ILE:HD11	1:A:494:VAL:HA	1.97	0.47
1:B:258:PHE:CE2	1:B:281:ALA:HA	2.50	0.47
1:A:581:GLU:HB3	1:A:582:PRO:CD	2.45	0.46
1:A:266:ARG:HD3	1:A:268:ILE:CD1	2.43	0.46
1:A:299:LEU:HD22	2:C:217:GLN:HG3	1.97	0.46
1:A:601:SER:O	1:A:604:GLU:HB2	2.16	0.46
1:B:202:ALA:HA	1:B:314:VAL:HG12	1.97	0.46
1:B:266:ARG:HD2	1:B:268:ILE:HD11	1.98	0.46
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.80	0.46
1:A:458:PHE:HA	1:A:461:TYR:CE2	2.51	0.46
1:A:231[B]:ARG:HH11	1:A:233:GLN:N	2.14	0.46
1:A:348:VAL:HG13	1:A:417:HIS:CD2	2.51	0.45
1:A:549:HIS:CE1	1:A:633:LEU:HD11	2.51	0.45
1:B:579:LEU:HD12	1:B:579:LEU:HA	1.78	0.45
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.98	0.45
1:A:226:GLU:CD	1:A:361:ARG:HH21	2.20	0.45
1:A:297:ARG:HG3	1:A:328:TYR:CE2	2.52	0.45
1:B:633:LEU:C	1:B:633:LEU:HD12	2.36	0.45
1:A:299:LEU:O	2:C:220:GLY:HA2	2.17	0.44
1:B:354[B]:ARG:HG3	1:B:413:VAL:HG11	1.99	0.44
1:B:354[A]:ARG:HB3	1:B:392[A]:GLU:OE2	2.16	0.44
1:A:182:MET:HG2	1:A:187:ARG:HB2	1.99	0.44
1:A:299:LEU:CD2	2:C:217:GLN:HG3	2.48	0.44
1:A:341:TYR:CE1	1:A:374:SER:HB3	2.53	0.44
1:B:435:ILE:HD12	1:B:492:ALA:HB1	1.99	0.44
1:A:459:MET:O	5:A:904:EDO:H12	2.18	0.44
1:A:358:ARG:NH2	6:A:2148:HOH:O	2.51	0.43
1:A:315:LEU:CD1	1:A:420:LEU:HD11	2.48	0.43
1:A:192:LEU:HD22	1:A:201:ARG:HG3	2.01	0.43
1:B:250:MET:O	1:B:254:GLU:HB2	2.19	0.43
1:B:297:ARG:HG3	1:B:328:TYR:CD2	2.53	0.43
1:B:467:SER:HA	1:B:474:ARG:NH2	2.33	0.43
1:A:481:VAL:O	1:A:485:VAL:HG23	2.18	0.43
1:B:185:LEU:HD22	1:B:241:LEU:HB2	1.99	0.43
2:C:214:CYS:CB	2:C:217:GLN:NE2	2.81	0.43
1:A:341:TYR:CZ	1:A:374:SER:HB3	2.54	0.43
1:A:387:LEU:C	1:A:387:LEU:HD23	2.39	0.43
1:A:505:PHE:HB2	5:B:903:EDO:H11	2.01	0.43
1:B:312:LEU:CD2	1:B:420:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ALA:HB1	1:A:567:LEU:HD11	2.01	0.42
1:B:458:PHE:HA	1:B:461:TYR:CE2	2.55	0.42
1:B:275:LEU:O	1:B:277:PRO:HD3	2.19	0.42
1:B:328:TYR:HB2	1:B:417:HIS:CE1	2.54	0.42
1:A:474:ARG:O	1:A:478:MET:HG2	2.19	0.42
1:B:265:ALA:HB1	1:B:272:ARG:NE	2.34	0.42
1:B:267:TYR:C	1:B:268:ILE:HG13	2.36	0.42
1:A:328:TYR:HB2	1:A:417:HIS:CE1	2.54	0.42
1:A:202:ALA:HA	1:A:314:VAL:HG12	2.01	0.41
1:B:309:TRP:CD1	1:B:309:TRP:C	2.92	0.41
1:A:428:TRP:CE2	1:B:480:LYS:HD3	2.55	0.41
1:B:444:MET:O	1:B:451:ARG:HD3	2.20	0.41
1:B:435:ILE:HD11	1:B:494:VAL:HA	2.02	0.41
1:B:503:LYS:HD2	1:B:568:TYR:CZ	2.56	0.41
1:A:224:GLU:HB2	5:A:903:EDO:H21	2.02	0.41
1:A:633:LEU:C	1:A:633:LEU:HD12	2.41	0.41
1:B:291:GLN:HA	1:B:291:GLN:OE1	2.21	0.41
1:A:213:MET:HA	1:A:214:PRO:HD3	1.90	0.41
1:B:202:ALA:HA	1:B:314:VAL:CG1	2.50	0.41
1:B:350:GLN:O	1:B:393:PRO:HA	2.21	0.41
1:B:435:ILE:HG22	1:B:436:LEU:N	2.35	0.41
1:A:592:ALA:O	1:A:596:GLU:HG3	2.21	0.40
1:A:523:VAL:HG12	6:A:2240:HOH:O	2.21	0.40
2:D:221:LYS:HB2	2:D:222:PRO:HD2	2.03	0.40
1:A:607:ARG:NH1	1:A:610:ASP:OD1	2.55	0.40
1:B:265:ALA:HB1	1:B:272:ARG:HE	1.86	0.40
1:A:447:ASN:OD1	1:A:487[B]:ARG:NH2	2.54	0.40
1:B:312:LEU:HD11	1:B:325:SER:HB3	2.04	0.40
1:A:555:ILE:O	1:A:569:TYR:HA	2.21	0.40
1:B:362:PRO:HD3	1:B:403:PHE:CE1	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	459/467 (98%)	450 (98%)	9 (2%)	0	100	100
1	B	461/467 (99%)	452 (98%)	9 (2%)	0	100	100
2	C	10/20 (50%)	9 (90%)	1 (10%)	0	100	100
2	D	10/20 (50%)	8 (80%)	2 (20%)	0	100	100
All	All	940/974 (96%)	919 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/399 (98%)	370 (95%)	21 (5%)	22	30
1	B	389/399 (98%)	374 (96%)	15 (4%)	32	46
2	C	8/17 (47%)	4 (50%)	4 (50%)	0	0
2	D	9/17 (53%)	8 (89%)	1 (11%)	6	7
All	All	797/832 (96%)	756 (95%)	41 (5%)	25	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	MET
1	A	216[A]	ASP
1	A	216[B]	ASP
1	A	260	GLN
1	A	268	ILE
1	A	273	GLU
1	A	280	ARG
1	A	297	ARG
1	A	318	GLN
1	A	354	ARG

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Mol	Chain	Res	Type
1	A	361	ARG
1	A	363	ARG
1	A	411	ASP
1	A	487[A]	ARG
1	A	487[B]	ARG
1	A	519	ARG
1	A	590	GLN
1	A	591	GLN
1	A	604	GLU
1	A	607	ARG
1	A	615	SER
1	B	216	ASP
1	B	252	ARG
1	B	271	ARG
1	B	273	GLU
1	B	288	SER
1	B	297	ARG
1	B	318	GLN
1	B	354[A]	ARG
1	B	354[B]	ARG
1	B	361	ARG
1	B	478	MET
1	B	529	ARG
1	B	583	LYS
1	B	601	SER
1	B	629	LYS
2	C	215	ASN
2	C	217	GLN
2	C	219	ILE
2	C	221	LYS
2	D	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	B	235	HIS
1	B	379	GLN
2	C	217	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	EDO	B	903	-	3,3,3	0.42	0	2,2,2	0.38	0
4	OGA	A	902	3	9,9,9	1.64	3 (33%)	10,11,11	1.64	1 (10%)
4	OGA	B	902	3	9,9,9	1.31	2 (22%)	10,11,11	1.59	2 (20%)
5	EDO	A	903	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	A	904	-	3,3,3	0.57	0	2,2,2	0.09	0
5	EDO	B	905	-	3,3,3	0.47	0	2,2,2	0.27	0
5	EDO	B	904	-	3,3,3	0.45	0	2,2,2	0.32	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
5	EDO	B	903	-	-	0/1/1/1	-
4	OGA	A	902	3	-	0/8/9/9	-
4	OGA	B	902	3	-	0/8/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	903	-	-	0/1/1/1	-
5	EDO	A	904	-	-	1/1/1/1	-
5	EDO	B	905	-	-	1/1/1/1	-
5	EDO	B	904	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	OGA	C2-C1	-3.43	1.49	1.54
4	B	902	OGA	C2-C1	-2.45	1.51	1.54
4	A	902	OGA	O2-C1	2.15	1.36	1.30
4	A	902	OGA	O2'-C2	-2.10	1.19	1.23
4	B	902	OGA	O2-C1	2.04	1.36	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	OGA	O2-C1-C2	2.85	121.54	113.15
4	A	902	OGA	O2-C1-C2	2.80	121.40	113.15
4	B	902	OGA	O2'-C2-N1	-2.00	119.63	123.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	905	EDO	O1-C1-C2-O2
5	A	904	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	903	EDO	1	0
5	A	903	EDO	1	0
5	A	904	EDO	1	0
5	B	904	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 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%)	0.39	14 (3%) 49 56	20, 35, 61, 70	2 (0%)
1	B	459/467 (98%)	0.38	15 (3%) 46 53	18, 34, 60, 70	2 (0%)
2	C	12/20 (60%)	2.69	7 (58%) 0 0	48, 59, 86, 93	3 (25%)
2	D	12/20 (60%)	2.14	6 (50%) 0 0	52, 59, 76, 79	3 (25%)
All	All	941/974 (96%)	0.43	42 (4%) 33 40	18, 35, 61, 93	10 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	214	CYS	6.6
1	A	639	ALA	6.5
2	D	214	CYS	5.6
2	C	213	GLY	5.5
1	A	533	GLY	5.5
1	B	640	LEU	5.2
1	B	639	ALA	4.8
2	C	212	GLY	4.7
1	B	539	GLY	3.9
1	B	540	ALA	3.7
1	B	532	ALA	3.6
1	B	538	VAL	3.5
2	D	223	SER	3.5
2	C	223	SER	3.3
2	D	213	GLY	3.2
1	A	271	ARG	3.2
1	A	640	LEU	3.2
1	A	562	GLY	3.1
1	B	564	HIS	3.1
1	A	535	PRO	2.9
1	A	411	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	636	MET	2.7
1	B	271	ARG	2.6
2	D	212	GLY	2.6
2	D	222	PRO	2.6
2	D	216	HIS	2.5
1	B	620	LEU	2.4
1	A	269	ASN	2.4
1	B	562	GLY	2.3
1	A	275	LEU	2.2
2	C	222	PRO	2.2
1	A	539	GLY	2.2
1	B	637	PRO	2.2
2	C	221	LYS	2.2
1	A	530	TRP	2.2
1	B	469	SER	2.1
2	C	216	HIS	2.1
1	B	543	THR	2.1
1	B	275	LEU	2.1
1	A	564	HIS	2.1
1	B	566	PHE	2.0
1	A	470	LYS	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 monosaccharides 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	EDO	A	904	4/4	0.77	0.24	76,76,76,77	0
5	EDO	B	905	4/4	0.90	0.22	33,37,38,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	903	4/4	0.92	0.25	33,36,37,41	0
4	OGA	B	902	10/10	0.94	0.13	25,29,31,32	0
5	EDO	B	903	4/4	0.94	0.21	39,40,40,41	0
4	OGA	A	902	10/10	0.94	0.14	26,30,34,36	0
5	EDO	B	904	4/4	0.95	0.13	32,33,33,34	0
3	MN	B	901	1/1	0.98	0.11	27,27,27,27	0
3	MN	A	901	1/1	0.98	0.10	24,24,24,24	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.