



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:32 AM BST

PDB ID : 4CCM
Title : 60S ribosomal protein L8 histidine hydroxylase (NO66) in complex with Mn(II), N-oxalylglycine (NOG) and 60S ribosomal protein L8 (RPL8 G220C) peptide fragment (complex-1)
Authors : Chowdhury, R.; Schofield, C.J.
Deposited on : 2013-10-23
Resolution : 2.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

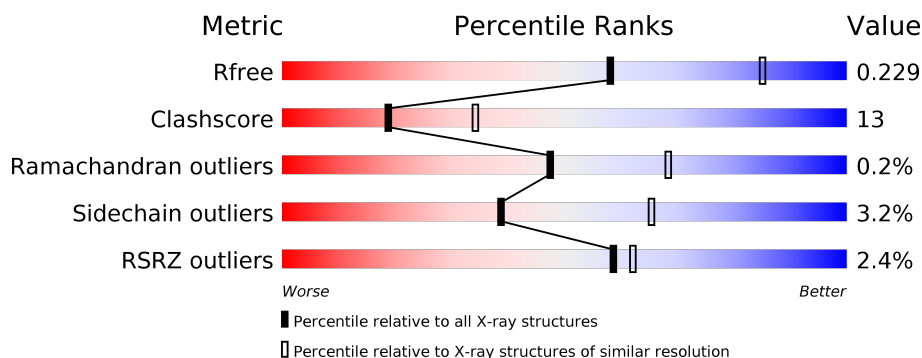
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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>2%</div> <div>69%</div> <div>28%</div> <div>••</div> </div>
1	B	467	<div> <div>%</div> <div>72%</div> <div>25%</div> <div>••</div> </div>
2	C	35	<div> <div>6%</div> <div>17%</div> <div>6%</div> <div>77%</div> </div>
2	D	35	<div> <div>14%</div> <div>11%</div> <div>17%</div> <div>69%</div> <div>•</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7841 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	457	Total	C	N	O	S	0	1	0
			3650	2322	644	668	16			
1	B	459	Total	C	N	O	S	0	1	0
			3670	2335	649	670	16			

There are 16 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
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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			63	38	14	10	1			
2	D	11	Total	C	N	O	S	0	0	0
			75	44	17	13	1			

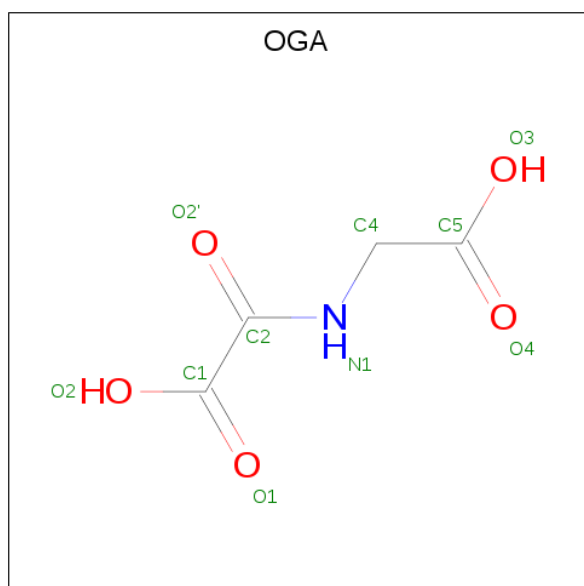
There are 2 discrepancies between the modelled and reference sequences:

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 1 1	0	0
3	A	1	Total Mn 1 1	0	0

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C₄H₅NO₅).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

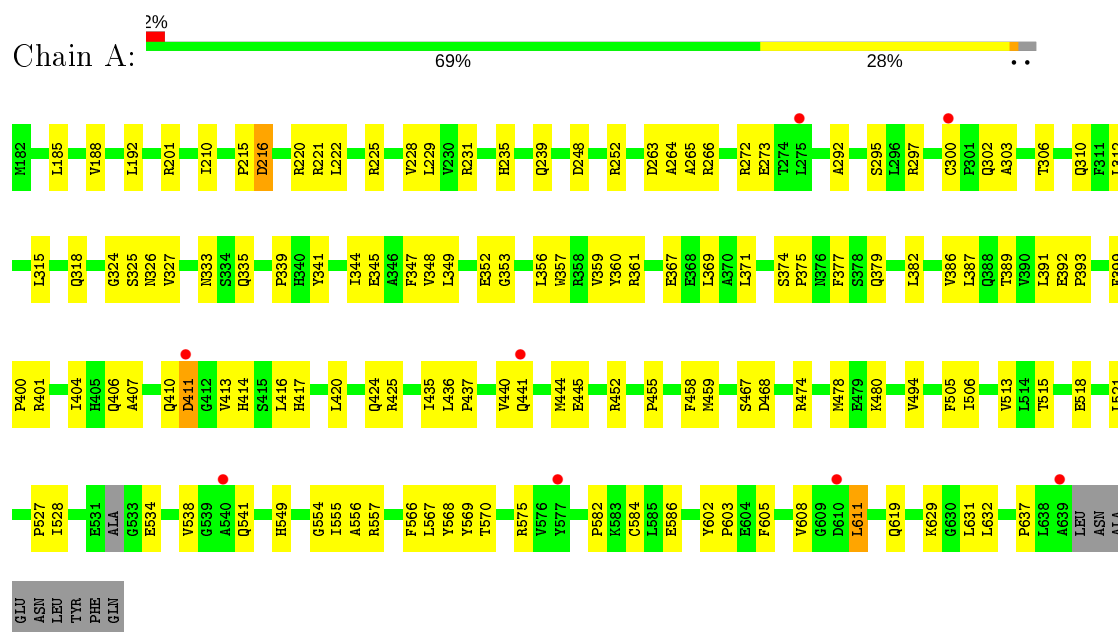
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total	O	0	0
			189	189		
6	B	159	Total	O	0	0
			159	159		
6	D	1	Total	O	0	0
			1	1		

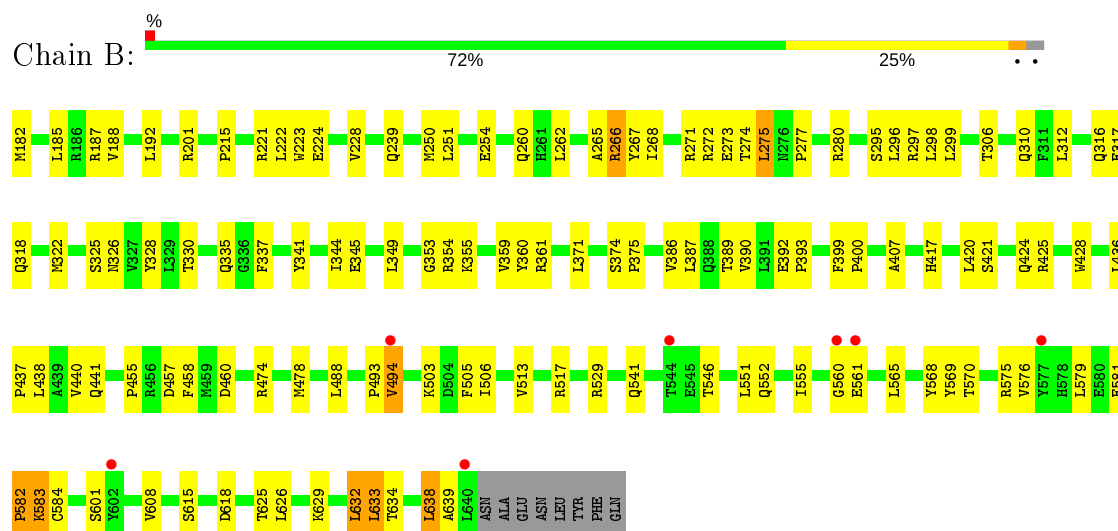
3 Residue-property plots

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.

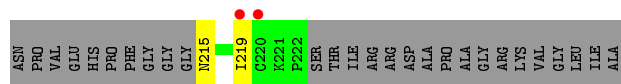
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66



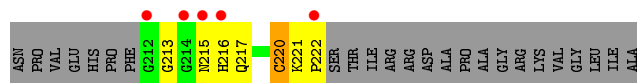
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66



- 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, α , β , γ	154.77Å 83.50Å 96.87Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	44.07 – 2.51 44.07 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.07-2.51) 98.8 (44.07-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.228 , 0.236 0.224 , 0.229	Depositor DCC
R_{free} test set	2071 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.41	0/3747	0.62	0/5100
1	B	0.42	0/3768	0.62	2/5129 (0.0%)
2	C	0.37	0/65	0.49	0/88
2	D	0.74	0/77	0.76	0/103
All	All	0.42	0/7657	0.62	2/10420 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	LEU	CB-CA-C	-5.80	99.18	110.20
1	B	639	ALA	N-CA-CB	-5.01	103.09	110.10

There are no chirality outliers.

There are no planarity outliers.

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	3650	0	3552	95	0
1	B	3670	0	3582	95	0
2	C	63	0	51	2	0
2	D	75	0	60	12	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	10	0	3	0	0
4	B	10	0	4	0	0
5	A	4	0	6	1	0
5	B	8	0	12	2	0
6	A	189	0	0	7	0
6	B	159	0	0	5	0
6	D	1	0	0	0	0
All	All	7841	0	7270	193	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 13.

All (193) 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:280[B]:ARG:CG	1:B:280[B]:ARG:HH11	1.73	1.01
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.57	0.86
1:B:280[B]:ARG:HG3	1:B:280[B]:ARG:HH11	1.43	0.82
1:B:280[B]:ARG:HG2	1:B:280[B]:ARG:HH11	1.48	0.79
2:D:221:LYS:H	2:D:222:PRO:HA	1.47	0.79
1:A:310:GLN:HG3	1:A:513:VAL:HG11	1.67	0.76
1:B:260:GLN:HA	2:D:222:PRO:HG3	1.69	0.74
1:A:216[B]:ASP:OD2	1:A:220:ARG:NH1	2.21	0.73
1:B:254:GLU:O	1:B:280[B]:ARG:NH2	2.24	0.71
1:A:266:ARG:HG2	1:A:273:GLU:HG3	1.71	0.69
1:A:608:VAL:O	1:A:611:LEU:HD23	1.92	0.68
1:B:280[B]:ARG:CG	1:B:280[B]:ARG:NH1	2.46	0.68
2:D:221:LYS:N	2:D:222:PRO:HA	2.09	0.67
1:B:251:LEU:O	1:B:280[B]:ARG:NH2	2.28	0.67
1:B:325:SER:C	1:B:326:ASN:HD22	1.99	0.66
1:B:297:ARG:HH11	1:B:299:LEU:HD21	1.60	0.65
1:A:216[B]:ASP:OD1	1:A:220:ARG:NH1	2.30	0.64
1:A:344:ILE:O	1:A:344:ILE:HD12	1.98	0.64
1:A:369:LEU:HA	1:A:401:ARG:HG3	1.81	0.62
1:B:345:GLU:OE1	1:B:400:PRO:HA	1.98	0.61
1:A:361:ARG:HH11	1:A:361:ARG:HB3	1.64	0.61
1:A:436:LEU:HB2	1:A:437:PRO:HD3	1.83	0.60
1:B:436:LEU:HB2	1:B:437:PRO:HD3	1.83	0.59
1:A:306:THR:HG22	1:A:575:ARG:HH12	1.67	0.58
1:A:216[B]:ASP:CG	1:A:220:ARG:NH1	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TRP:CD1	1:B:224:GLU:HG3	2.39	0.58
1:B:275:LEU:HD23	1:B:275:LEU:N	2.18	0.58
1:A:265:ALA:HB1	1:A:272:ARG:HE	1.68	0.57
1:B:280[B]:ARG:NH1	1:B:280[B]:ARG:HG3	2.14	0.57
1:B:546:THR:O	1:B:608:VAL:HG23	2.03	0.57
1:A:455:PRO:HB2	1:A:458:PHE:HB3	1.86	0.57
1:A:474:ARG:O	1:A:478:MET:HG2	2.05	0.57
1:B:299:LEU:HD22	2:D:217:GLN:HB2	1.87	0.57
1:B:361:ARG:NE	6:B:2025:HOH:O	2.30	0.56
1:A:452:ARG:HD3	5:A:903:EDO:H22	1.86	0.56
1:B:306:THR:HG22	1:B:575:ARG:NH1	2.20	0.56
1:A:505:PHE:HB2	5:B:903:EDO:H11	1.87	0.56
1:B:349:LEU:O	1:B:417:HIS:HB2	2.05	0.56
1:A:306:THR:HG22	1:A:575:ARG:NH1	2.20	0.56
1:A:229:LEU:HD22	1:A:389:THR:HG21	1.89	0.55
1:B:353:GLY:O	1:B:393:PRO:HD3	2.05	0.55
1:B:306:THR:HG22	1:B:575:ARG:HH12	1.71	0.55
1:A:333:ASN:HD21	1:A:411:ASP:HA	1.71	0.55
1:B:260:GLN:HG2	2:D:222:PRO:HG3	1.88	0.55
1:B:615:SER:HB3	1:B:618:ASP:OD2	2.07	0.55
1:A:302:GLN:HB3	1:A:312:LEU:HD12	1.89	0.55
1:A:361:ARG:HB3	1:A:361:ARG:NH1	2.22	0.55
1:A:441:GLN:O	1:A:445:GLU:HG3	2.07	0.54
1:A:568:TYR:CD1	1:A:584:CYS:HB3	2.42	0.54
1:B:359:VAL:O	1:B:386:VAL:HG12	2.08	0.54
1:B:185:LEU:O	1:B:188:VAL:HG12	2.07	0.54
1:B:312:LEU:CD2	1:B:420:LEU:HD13	2.37	0.53
1:A:297:ARG:HA	1:A:327:VAL:O	2.08	0.53
1:A:602:TYR:CE1	1:A:603:PRO:HG3	2.42	0.53
1:B:280[B]:ARG:NH1	1:B:280[B]:ARG:HG2	2.19	0.52
1:B:297:ARG:HH21	1:B:337:PHE:HE2	1.57	0.52
1:B:335:GLN:HG3	1:B:407:ALA:O	2.09	0.52
1:A:555:ILE:O	1:A:569:TYR:HA	2.09	0.52
1:A:341:TYR:CZ	1:A:374:SER:HB3	2.45	0.52
1:A:444:MET:HB3	1:B:371:LEU:HD11	1.91	0.52
1:A:379:GLN:HE22	1:A:406:GLN:HE22	1.58	0.52
1:A:248:ASP:O	1:A:252:ARG:HG3	2.10	0.52
2:D:220:CYS:SG	2:D:220:CYS:O	2.67	0.52
1:A:361:ARG:HG3	1:A:386:VAL:HB	1.92	0.52
1:A:353:GLY:O	1:A:393:PRO:HD3	2.10	0.51
1:B:551:LEU:O	1:B:552:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ILE:O	1:B:569:TYR:HA	2.11	0.51
1:B:424:GLN:HG2	1:B:425:ARG:HG2	1.93	0.51
1:A:333:ASN:ND2	1:A:411:ASP:HA	2.25	0.51
1:A:339:PRO:HG2	1:A:377:PHE:O	2.10	0.51
1:B:581:GLU:O	1:B:583:LYS:HG2	2.11	0.51
1:B:626:LEU:HB3	1:B:632:LEU:HD13	1.92	0.51
1:B:633:LEU:HD12	1:B:633:LEU:C	2.30	0.51
1:A:349:LEU:O	1:A:417:HIS:HB2	2.11	0.51
1:A:382:LEU:CD2	1:A:404:ILE:HG21	2.41	0.51
1:A:459:MET:HE2	6:A:2126:HOH:O	2.11	0.51
1:B:222:LEU:HD13	1:B:228:VAL:HG21	1.93	0.51
1:B:275:LEU:HD23	1:B:275:LEU:H	1.76	0.51
1:B:387:LEU:HD21	1:B:389:THR:HG22	1.91	0.50
1:B:192:LEU:O	1:B:201:ARG:HD3	2.11	0.50
1:A:382:LEU:HD21	1:A:404:ILE:HG21	1.93	0.50
1:A:359:VAL:O	1:A:386:VAL:HG12	2.12	0.50
1:B:267:TYR:C	1:B:268:ILE:HG13	2.32	0.50
1:B:506:ILE:O	1:B:570:THR:HG22	2.11	0.49
1:A:352:GLU:HG3	1:A:416:LEU:HD23	1.93	0.49
1:B:182:MET:O	1:B:187:ARG:NH1	2.46	0.49
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.48	0.49
1:B:266:ARG:HG3	1:B:273:GLU:CG	2.43	0.49
1:A:266:ARG:HG2	1:A:273:GLU:CG	2.40	0.49
1:A:554:GLY:HA2	6:A:2164:HOH:O	2.12	0.49
1:B:344:ILE:HG12	1:B:421:SER:HB2	1.94	0.49
1:A:222:LEU:HD13	1:A:228:VAL:HG21	1.95	0.48
1:B:262:LEU:HD11	1:B:296:LEU:HB3	1.95	0.48
1:B:328:TYR:HB2	1:B:417:HIS:CE1	2.48	0.48
1:A:424:GLN:HG2	1:A:425:ARG:HG2	1.96	0.48
1:A:478:MET:SD	1:B:494:VAL:HG21	2.54	0.48
1:B:625:THR:HG23	6:B:2155:HOH:O	2.13	0.48
1:B:438:LEU:HB3	1:B:493:PRO:HG3	1.96	0.48
1:B:505:PHE:HB2	5:B:904:EDO:H11	1.94	0.48
1:B:310:GLN:CA	1:B:513:VAL:HG21	2.37	0.48
1:B:455:PRO:HB2	1:B:458:PHE:HB3	1.94	0.48
1:B:581:GLU:HB3	1:B:582:PRO:HD2	1.96	0.48
1:A:265:ALA:HB1	1:A:272:ARG:NE	2.29	0.47
1:B:265:ALA:HB1	1:B:272:ARG:HE	1.78	0.47
1:A:348:VAL:HG13	1:A:417:HIS:CD2	2.49	0.47
1:A:185:LEU:O	1:A:188:VAL:HG12	2.14	0.47
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ALA:HB1	1:A:567:LEU:HD11	1.95	0.47
1:A:325:SER:O	1:A:326:ASN:ND2	2.48	0.47
1:B:266:ARG:HG3	1:B:273:GLU:HG3	1.96	0.47
1:B:541:GLN:HA	6:B:2129:HOH:O	2.15	0.47
1:B:576:VAL:HB	1:B:579:LEU:HB2	1.96	0.47
1:A:265:ALA:HB2	1:A:272:ARG:HH21	1.80	0.46
1:A:315:LEU:HD12	1:A:420:LEU:HD11	1.97	0.46
1:B:355:LYS:O	1:B:390:VAL:HA	2.14	0.46
1:B:223:TRP:NE1	1:B:224:GLU:HG3	2.30	0.46
1:A:324:GLY:O	1:A:325:SER:HB2	2.15	0.46
1:B:354:ARG:NH2	1:B:392:GLU:HG2	2.31	0.46
1:A:345:GLU:OE1	1:A:400:PRO:HA	2.16	0.46
1:B:360:TYR:CD1	1:B:360:TYR:N	2.84	0.46
6:A:2075:HOH:O	2:C:215:ASN:HB3	2.15	0.46
1:A:557:ARG:HD2	6:A:2166:HOH:O	2.15	0.46
1:B:634:THR:HG21	1:B:638:LEU:HD21	1.99	0.45
1:A:266:ARG:NH2	1:A:292:ALA:O	2.50	0.45
1:B:399:PHE:HA	1:B:400:PRO:HD3	1.70	0.45
1:B:506:ILE:HG23	1:B:570:THR:HG23	1.99	0.45
1:B:215:PRO:HD2	6:B:2017:HOH:O	2.17	0.45
1:B:274:THR:OG1	2:D:213:GLY:HA3	2.16	0.45
1:B:295:SER:OG	1:B:330:THR:HG23	2.16	0.45
1:B:474:ARG:O	1:B:478:MET:HG2	2.17	0.45
1:A:440:VAL:O	1:A:444:MET:HG3	2.16	0.45
1:A:410:GLN:HB2	6:A:2108:HOH:O	2.15	0.44
1:B:260:GLN:HG2	2:D:222:PRO:CD	2.47	0.44
1:B:601:SER:HB2	6:B:2151:HOH:O	2.16	0.44
1:A:515:THR:OG1	1:A:518:GLU:HG3	2.17	0.44
1:B:260:GLN:CA	2:D:222:PRO:HG3	2.43	0.44
1:A:506:ILE:O	1:A:570:THR:HG22	2.18	0.44
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.98	0.44
1:B:221:ARG:HG3	1:B:221:ARG:HH11	1.83	0.44
1:B:568:TYR:CD2	1:B:584:CYS:HB3	2.53	0.44
1:A:235:HIS:HD2	6:A:2035:HOH:O	2.00	0.44
2:D:221:LYS:N	2:D:222:PRO:CA	2.79	0.44
1:A:467:SER:HA	1:A:474:ARG:NH2	2.33	0.44
1:A:528:ILE:HD12	1:A:538:VAL:HA	2.00	0.44
1:B:374:SER:HB2	1:B:375:PRO:HD2	1.98	0.44
1:B:387:LEU:C	1:B:387:LEU:HD23	2.38	0.44
1:A:436:LEU:HD11	1:B:488:LEU:HD11	1.99	0.44
1:A:210:ILE:HD11	1:A:215:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:O	1:B:277:PRO:HD3	2.18	0.44
1:A:608:VAL:C	1:A:611:LEU:HD23	2.37	0.43
1:B:250:MET:SD	1:B:298:LEU:HD21	2.58	0.43
1:A:611:LEU:H	1:A:619:GLN:NE2	2.16	0.43
1:B:260:GLN:HG2	2:D:222:PRO:CG	2.48	0.43
1:A:387:LEU:HD21	1:A:389:THR:HG22	2.00	0.43
1:A:582:PRO:HB3	6:A:2143:HOH:O	2.18	0.43
1:A:549:HIS:CD2	1:A:605:PHE:CE1	3.07	0.43
1:B:581:GLU:OE1	1:B:581:GLU:HA	2.18	0.43
1:A:192:LEU:O	1:A:201:ARG:HD2	2.19	0.43
1:B:440:VAL:HG13	1:B:441:GLN:N	2.34	0.43
1:A:264:ALA:HA	1:A:295:SER:O	2.19	0.43
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.72	0.43
1:B:266:ARG:HD2	1:B:268:ILE:HD12	2.00	0.43
1:B:560:GLY:O	1:B:561:GLU:HG3	2.19	0.43
1:A:413:VAL:HG22	1:A:414:HIS:N	2.34	0.42
1:A:480:LYS:HD3	1:B:428:TRP:CZ2	2.54	0.42
1:B:560:GLY:HA2	1:B:565:LEU:HD23	2.01	0.42
1:B:503:LYS:HE3	1:B:568:TYR:CE2	2.55	0.42
1:A:335:GLN:HG3	1:A:407:ALA:O	2.20	0.42
1:A:360:TYR:CD1	1:A:360:TYR:N	2.88	0.42
1:A:357:TRP:CD1	1:A:391:LEU:HD12	2.54	0.42
1:A:629:LYS:HB3	1:A:631:LEU:HG	2.02	0.42
1:A:566:PHE:CE1	1:A:586:GLU:HG3	2.55	0.42
1:B:188:VAL:O	1:B:192:LEU:HG	2.19	0.42
1:B:316:GLN:HG3	1:B:317:GLU:N	2.35	0.41
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.89	0.41
1:B:581:GLU:HB3	1:B:582:PRO:CD	2.49	0.41
2:D:215:ASN:O	2:D:216:HIS:C	2.58	0.41
2:C:219:ILE:O	2:C:219:ILE:HG13	2.19	0.41
1:B:506:ILE:HG23	1:B:570:THR:CG2	2.50	0.41
1:A:356:LEU:O	1:A:407:ALA:HA	2.20	0.41
1:B:457:ASP:O	1:B:460:ASP:HB2	2.20	0.41
1:A:300:CYS:SG	1:A:303:ALA:HB2	2.60	0.41
1:A:549:HIS:C	1:A:632:LEU:HD12	2.41	0.41
1:B:438:LEU:CB	1:B:493:PRO:HG3	2.50	0.41
1:A:521:LEU:HD23	1:A:637:PRO:HG3	2.02	0.41
1:A:371:LEU:HD22	1:A:425:ARG:HH12	1.85	0.41
1:A:188:VAL:O	1:A:192:LEU:HG	2.21	0.41
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.86	0.41
1:A:347:PHE:HB2	1:A:420:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:HD11	1:A:494:VAL:HA	2.03	0.40
1:A:549:HIS:HD2	1:A:605:PHE:CD1	2.39	0.40
1:A:341:TYR:CE2	1:A:367:GLU:HG2	2.56	0.40
1:A:374:SER:HB2	1:A:375:PRO:HD2	2.04	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	454/467 (97%)	432 (95%)	21 (5%)	1 (0%)	47	68
1	B	458/467 (98%)	436 (95%)	21 (5%)	1 (0%)	47	68
2	C	6/35 (17%)	5 (83%)	1 (17%)	0	100	100
2	D	9/35 (26%)	6 (67%)	3 (33%)	0	100	100
All	All	927/1004 (92%)	879 (95%)	46 (5%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	PRO
1	B	582	PRO

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	386/400 (96%)	374 (97%)	12 (3%)	40	67
1	B	388/400 (97%)	375 (97%)	13 (3%)	37	63
2	C	7/27 (26%)	7 (100%)	0	100	100
2	D	7/27 (26%)	6 (86%)	1 (14%)	3	6
All	All	788/854 (92%)	762 (97%)	26 (3%)	39	64

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216[A]	ASP
1	A	216[B]	ASP
1	A	231	ARG
1	A	239	GLN
1	A	263	ASP
1	A	318	GLN
1	A	392	GLU
1	A	411	ASP
1	A	468	ASP
1	A	534	GLU
1	A	541	GLN
1	A	611	LEU
1	B	239	GLN
1	B	266	ARG
1	B	271	ARG
1	B	275	LEU
1	B	318	GLN
1	B	322	MET
1	B	494	VAL
1	B	517	ARG
1	B	529	ARG
1	B	583	LYS
1	B	629	LYS
1	B	632	LEU
1	B	633	LEU
2	D	220	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	257	GLN
1	A	260	GLN
1	A	310	GLN
1	A	318	GLN
1	A	326	ASN
1	A	379	GLN
1	A	465	GLN
1	A	466	HIS
1	A	537	ASN
1	A	541	GLN
1	A	564	HIS
1	A	591	GLN
1	A	619	GLN
1	B	257	GLN
1	B	333	ASN
1	B	410	GLN
1	B	591	GLN
2	D	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 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	$\# Z > 2$
4	OGA	B	902	3	3,9,9	0.91	0	4,11,11	1.96	1 (25%)
4	OGA	A	902	3	3,9,9	1.19	0	4,11,11	2.00	1 (25%)
5	EDO	A	903	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	B	903	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	B	904	-	3,3,3	0.47	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
4	OGA	B	902	3	-	0/3/9/9	-
4	OGA	A	902	3	-	0/3/9/9	-
5	EDO	A	903	-	-	1/1/1/1	-
5	EDO	B	903	-	-	0/1/1/1	-
5	EDO	B	904	-	-	0/1/1/1	-

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	3.91	119.48	115.60
4	B	902	OGA	C1-C2-N1	3.74	119.31	115.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	903	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/467 (97%)	0.23	8 (1%) 68 71	31, 52, 92, 100	2 (0%)
1	B	459/467 (98%)	0.22	7 (1%) 73 75	27, 51, 88, 100	2 (0%)
2	C	8/35 (22%)	1.44	2 (25%) 0 0	82, 92, 100, 100	0
2	D	11/35 (31%)	1.84	5 (45%) 0 0	77, 82, 100, 100	0
All	All	935/1004 (93%)	0.26	22 (2%) 59 62	27, 52, 93, 100	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	LEU	6.3
1	A	275	LEU	3.7
1	A	577	TYR	3.7
2	D	216	HIS	3.4
1	B	561	GLU	2.9
1	A	639	ALA	2.8
1	B	602	TYR	2.7
2	D	215	ASN	2.7
1	A	540	ALA	2.6
1	A	411	ASP	2.6
2	C	219	ILE	2.6
2	C	220	CYS	2.4
1	B	577	TYR	2.4
2	D	222	PRO	2.2
2	D	214	GLY	2.2
1	A	300	CYS	2.2
2	D	212	GLY	2.1
1	B	494	VAL	2.1
1	B	560	GLY	2.1
1	B	544	THR	2.0
1	A	610	ASP	2.0
1	A	441	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	903	4/4	0.89	0.24	66,68,69,71	0
4	OGA	A	902	10/10	0.94	0.16	41,43,50,50	0
4	OGA	B	902	10/10	0.96	0.14	37,42,50,51	0
5	EDO	B	904	4/4	0.96	0.17	45,49,49,50	0
5	EDO	B	903	4/4	0.97	0.17	49,51,52,53	0
3	MN	A	901	1/1	0.99	0.12	38,38,38,38	0
3	MN	B	901	1/1	0.99	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.