



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2014 – 06:41 AM EDT

PDB ID : 4CCK
Title : 60S ribosomal protein L8 histidine hydroxylase (NO66) in complex with Mn(II) and N-oxalylglycine (NOG)
Authors : Chowdhury, R.; Ge, W.; Clifton, I.J.; Schofield, C.J.
Deposited on : 2013-10-23
Resolution : 2.15 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

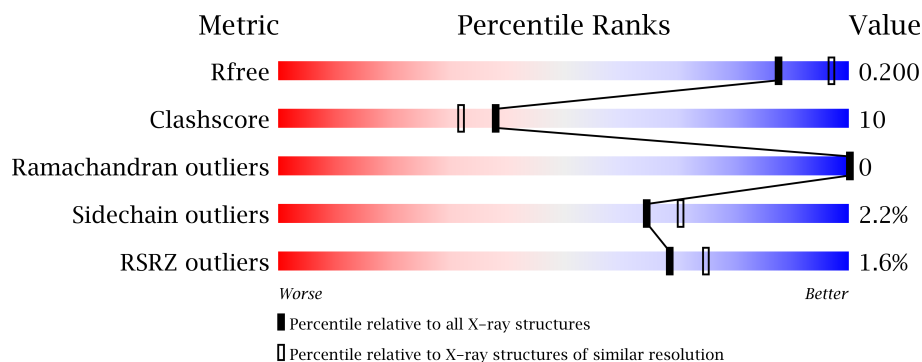
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.15 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	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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. 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	
1	C	467	
1	D	467	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MN	A	901	-	X
2	MN	B	901	-	X
2	MN	C	901	-	X
2	MN	D	901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	B	903	-	X
4	EDO	C	903	-	X
4	EDO	D	903	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15509 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	456	Total	C	N	O	S	0	2	0
			3662	2330	648	668	16			
1	B	456	Total	C	N	O	S	0	4	0
			3641	2329	637	659	16			
1	C	458	Total	C	N	O	S	0	4	0
			3663	2336	641	670	16			
1	D	459	Total	C	N	O	S	0	3	0
			3654	2331	639	668	16			

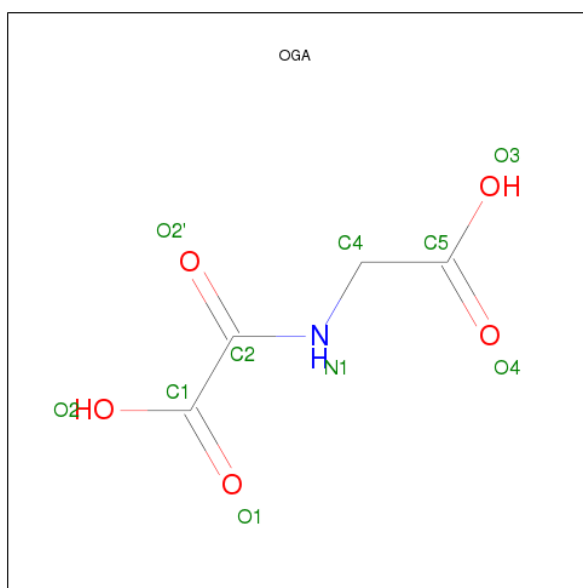
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
A	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3
B	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
B	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3
C	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
C	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3
D	182	MET	-	EXPRESSION TAG	UNP Q9H6W3
D	364	ALA	VAL	ENGINEERED MUTATION	UNP Q9H6W3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

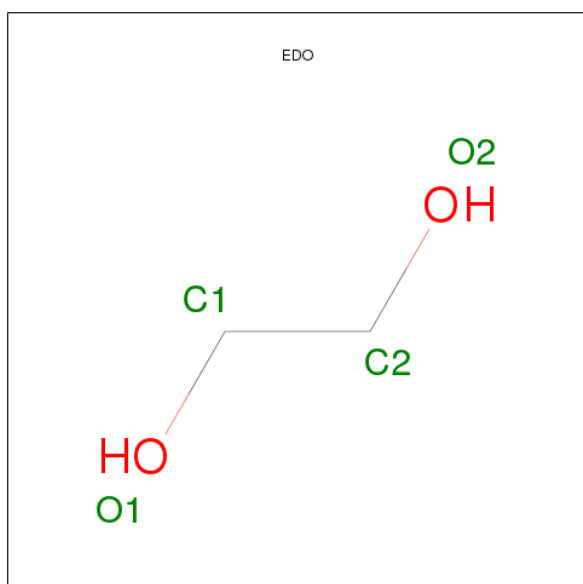
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

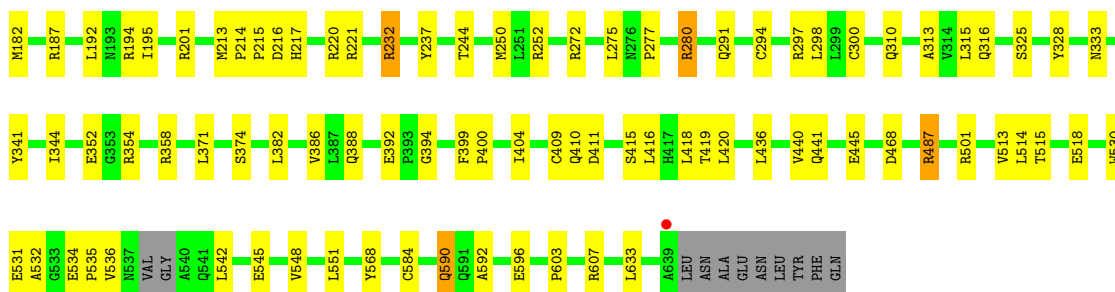
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	278	Total O 278 278	0	0
5	B	170	Total O 170 170	0	0
5	C	236	Total O 236 236	0	0
5	D	145	Total O 145 145	0	0

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.

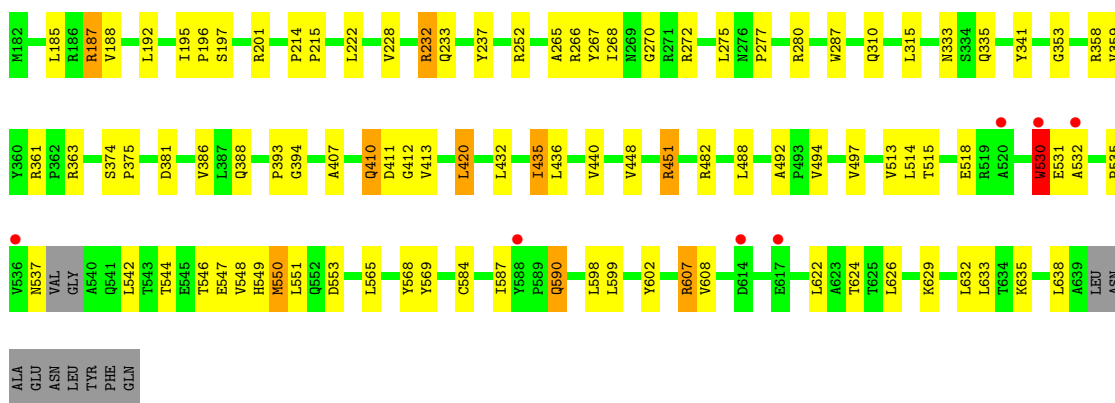
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

Chain A: 



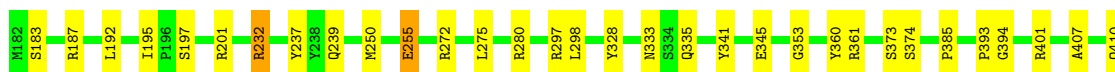
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

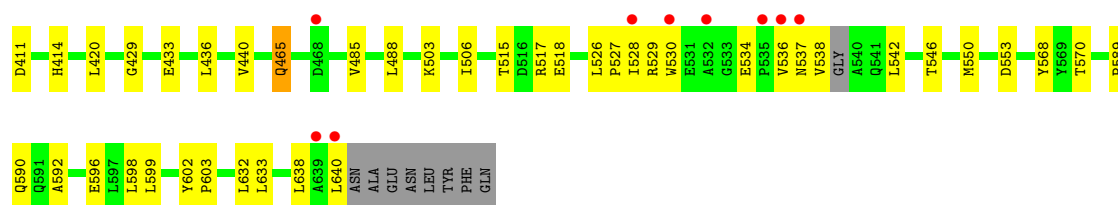
Chain B: 



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

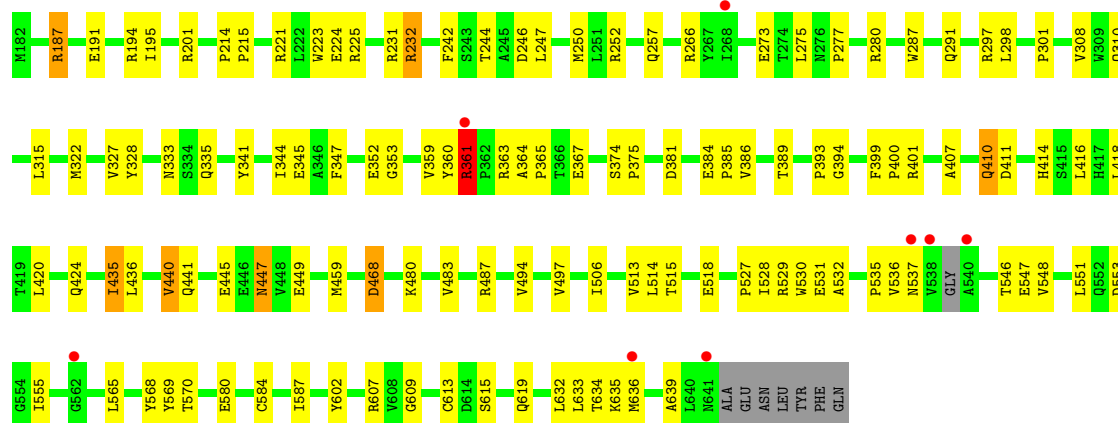
Chain C: 





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

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.41Å 80.71Å 151.54Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	81.10 – 2.15 81.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.9 (81.10-2.15) 98.8 (81.10-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.16Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.186 , 0.197 0.196 , 0.200	Depositor DCC
R_{free} test set	6595 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 131064 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, 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	0.35	0/3762	0.62	1/5117 (0.0%)
1	B	0.38	0/3749	0.59	1/5106 (0.0%)
1	C	0.35	0/3769	0.61	1/5131 (0.0%)
1	D	0.32	0/3757	0.58	2/5116 (0.0%)
All	All	0.35	0/15037	0.60	5/20470 (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	2
1	B	0	2
1	C	0	1
1	D	0	4
All	All	0	9

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361[A]	ARG	CB-CA-C	-5.92	98.57	110.40
1	D	361[B]	ARG	CB-CA-C	-5.92	98.57	110.40
1	A	548	VAL	CB-CA-C	-5.83	100.32	111.40
1	B	412	GLY	N-CA-C	5.74	127.45	113.10
1	C	632	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	487[A]	ARG	Mainchain
1	A	487[B]	ARG	Mainchain
1	B	530[A]	TRP	Mainchain
1	B	530[B]	TRP	Mainchain
1	C	465[B]	GLN	Mainchain
1	D	187[A]	ARG	Mainchain
1	D	187[B]	ARG	Mainchain
1	D	361[A]	ARG	Mainchain
1	D	361[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	3662	0	3583	67	0
1	B	3641	0	3554	87	0
1	C	3663	0	3571	63	0
1	D	3654	0	3553	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	3	0	0
3	B	10	0	3	0	0
3	C	10	0	3	0	0
3	D	10	0	3	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	278	0	0	7	0
5	B	170	0	0	2	0
5	C	236	0	0	2	0
5	D	145	0	0	4	0
All	All	15509	0	14297	288	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 10.

All (288) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:448:VAL:HG23	1:B:451:ARG:HH12	1.34	0.93
1:A:232:ARG:HD2	1:A:394:GLY:O	1.82	0.80
1:C:529:ARG:O	1:C:536:VAL:HG12	1.82	0.79
1:B:515:THR:OG1	1:B:518:GLU:HG3	1.83	0.79
1:B:252:ARG:HH22	1:D:528:ILE:HD13	1.51	0.74
1:D:247:LEU:HA	1:D:250:MET:HE2	1.68	0.73
1:B:410:GLN:HA	1:B:410:GLN:HE21	1.56	0.71
1:B:550:MET:HE1	1:B:598:LEU:HB3	1.72	0.71
1:C:542:LEU:HD22	1:C:546:THR:HG21	1.72	0.70
1:C:436:LEU:HD12	1:D:440[B]:VAL:HG21	1.72	0.70
1:D:436:LEU:O	1:D:440[B]:VAL:HG23	1.91	0.70
1:D:242:PHE:HZ	1:D:250:MET:HE1	1.57	0.70
1:A:232:ARG:HD3	1:A:237:TYR:CD2	2.27	0.69
1:C:232:ARG:HD2	1:C:394:GLY:O	1.93	0.69
1:B:542:LEU:HD23	1:B:542:LEU:H	1.57	0.69
1:A:410:GLN:HE21	1:A:410:GLN:HA	1.57	0.69
1:D:506:ILE:HG23	1:D:570:THR:HG22	1.76	0.66
1:D:410:GLN:HA	1:D:410:GLN:HE21	1.61	0.65
1:B:448:VAL:HG23	1:B:451:ARG:NH1	2.10	0.65
1:A:436:LEU:HD13	1:B:436:LEU:HB3	1.78	0.65
1:B:353:GLY:O	1:B:393:PRO:HD3	1.96	0.65
1:A:280:ARG:HD3	5:A:2053:HOH:O	1.96	0.64
1:C:592:ALA:O	1:C:596:GLU:HG3	1.98	0.64
1:B:435:ILE:HD12	1:B:497:VAL:HG21	1.80	0.64
1:C:465[A]:GLN:HG2	5:C:2160:HOH:O	1.97	0.63
1:C:436:LEU:CD1	1:D:440[B]:VAL:CG2	2.77	0.63
1:C:589:PRO:HD2	1:C:590:GLN:HE22	1.65	0.62
1:D:487:ARG:HD2	5:D:2108:HOH:O	1.99	0.62
1:B:569:TYR:OH	1:B:629:LYS:HE2	1.98	0.62
1:C:232:ARG:HD3	1:C:237:TYR:CD2	2.34	0.62
1:C:353:GLY:O	1:C:393:PRO:HD3	2.00	0.61
1:C:436:LEU:O	1:C:440:VAL:HG23	2.01	0.61
1:D:515:THR:OG1	1:D:518:GLU:HG3	2.00	0.61
1:B:435:ILE:HG12	1:B:492:ALA:HB1	1.83	0.61
1:B:333:ASN:ND2	1:B:411:ASP:HA	2.16	0.61
1:B:547:GLU:HB2	1:B:635:LYS:HB2	1.82	0.61
1:B:335:GLN:HG3	1:B:407:ALA:O	2.02	0.60
1:D:435:ILE:HD11	1:D:494:VAL:HA	1.84	0.60
1:A:534:GLU:OE2	1:C:414:HIS:HD2	1.85	0.59
1:D:335:GLN:HG3	1:D:407:ALA:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:436:LEU:HD12	1:D:440[B]:VAL:CG2	2.33	0.59
1:C:550:MET:HE3	1:C:599:LEU:HD23	1.83	0.59
1:C:542:LEU:HD23	1:C:638:LEU:HD21	1.84	0.59
1:A:195:ILE:HB	1:A:201:ARG:HG2	1.85	0.59
1:A:371:LEU:HG	1:B:451:ARG:HD3	1.85	0.58
1:C:436:LEU:CD1	1:D:440[B]:VAL:HG22	2.33	0.58
1:A:592:ALA:O	1:A:596:GLU:HG3	2.04	0.58
1:B:232:ARG:HD2	1:B:394:GLY:O	2.04	0.57
1:B:435:ILE:HD12	1:B:497:VAL:CG2	2.34	0.57
1:B:542:LEU:HA	1:B:638:LEU:HD11	1.86	0.57
1:D:353:GLY:O	1:D:393:PRO:HD3	2.05	0.57
1:B:413:VAL:HG13	5:B:2084:HOH:O	2.04	0.57
1:A:440:VAL:HG21	1:B:436:LEU:HD12	1.87	0.57
1:C:436:LEU:HD11	1:D:440[B]:VAL:HG22	1.87	0.57
1:A:232:ARG:HD3	1:A:237:TYR:CG	2.41	0.56
1:D:364:ALA:HB1	1:D:365:PRO:HD2	1.87	0.56
1:B:361:ARG:HG3	1:B:386:VAL:HB	1.87	0.56
1:B:275:LEU:O	1:B:277:PRO:HD3	2.05	0.56
1:D:322:MET:HE2	5:D:2075:HOH:O	2.06	0.56
1:D:441:GLN:O	1:D:445:GLU:HG3	2.06	0.56
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.71	0.55
1:B:514:LEU:HD21	1:B:551:LEU:HD21	1.88	0.55
1:C:436:LEU:HD11	1:D:440[A]:VAL:HG13	1.88	0.55
1:B:451:ARG:HB2	1:B:451:ARG:HH11	1.72	0.55
1:B:530[A]:TRP:CZ3	1:B:535:PRO:HD3	2.40	0.55
1:D:347:PHE:HB2	1:D:420:LEU:HB3	1.88	0.55
1:A:313:ALA:O	1:A:316:GLN:HG2	2.07	0.55
1:B:268:ILE:HD11	5:B:2051:HOH:O	2.06	0.55
1:B:451:ARG:CB	1:B:451:ARG:HH11	2.20	0.55
1:B:590:GLN:H	1:B:590:GLN:CD	2.09	0.54
1:C:550:MET:HE2	1:C:598:LEU:HB3	1.88	0.54
1:C:440:VAL:HG21	1:D:436:LEU:HD12	1.88	0.54
1:D:547:GLU:HB2	1:D:635:LYS:HB2	1.89	0.54
1:A:514:LEU:HD21	1:A:551:LEU:HD21	1.90	0.54
1:D:615:SER:O	1:D:619:GLN:HB2	2.07	0.54
1:B:550:MET:HE1	1:B:598:LEU:CB	2.37	0.53
1:D:352:GLU:HB2	1:D:416:LEU:HB3	1.90	0.53
1:D:341:TYR:CZ	1:D:374:SER:HB3	2.44	0.53
1:D:506:ILE:HG23	1:D:570:THR:CG2	2.39	0.53
1:A:341:TYR:CZ	1:A:374:SER:HB3	2.45	0.52
1:D:548:VAL:HG12	1:D:634:THR:HG22	1.91	0.52
1:B:222:LEU:HD13	1:B:228:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.91	0.52
1:C:255:GLU:OE1	1:C:280:ARG:HD2	2.09	0.52
1:B:267:TYR:C	1:B:268:ILE:HD12	2.30	0.52
1:B:333:ASN:OD1	1:B:411:ASP:HA	2.10	0.52
1:C:275:LEU:HD12	1:C:275:LEU:N	2.25	0.52
1:A:358:ARG:HG2	1:A:388:GLN:HG3	1.92	0.52
1:C:553:ASP:HB2	1:C:602:TYR:CE1	2.44	0.52
1:D:514:LEU:HD21	1:D:551:LEU:HD21	1.92	0.51
1:A:436:LEU:HD11	1:B:488:LEU:HD13	1.92	0.51
1:A:182:MET:CE	1:A:187:ARG:HH11	2.23	0.51
1:B:530[B]:TRP:HZ2	1:D:414:HIS:NE2	2.08	0.51
1:B:333:ASN:CG	1:B:411:ASP:HA	2.30	0.51
1:C:515:THR:OG1	1:C:518:GLU:HG3	2.10	0.51
1:D:333:ASN:ND2	1:D:411:ASP:HA	2.26	0.51
1:C:590:GLN:H	1:C:590:GLN:NE2	2.08	0.51
1:D:363:ARG:NH1	1:D:381:ASP:HB3	2.26	0.51
1:A:354[A]:ARG:CZ	1:A:392:GLU:OE2	2.58	0.51
1:B:363:ARG:NH1	1:B:381:ASP:HB3	2.26	0.51
1:D:613:CYS:SG	1:D:619:GLN:HA	2.50	0.51
1:D:232:ARG:HD3	1:D:394:GLY:O	2.11	0.51
1:C:232:ARG:HD3	1:C:237:TYR:CG	2.46	0.50
1:C:361[A]:ARG:HH11	1:C:361[A]:ARG:HG2	1.75	0.50
1:D:301:PRO:HG2	1:D:327:VAL:HG23	1.93	0.50
1:A:410:GLN:NE2	1:A:410:GLN:HA	2.24	0.50
1:B:232:ARG:HD3	1:B:237:TYR:CD2	2.46	0.50
1:D:275:LEU:N	1:D:275:LEU:HD12	2.26	0.50
1:B:436:LEU:O	1:B:440[B]:VAL:HG23	2.12	0.50
1:B:622:LEU:O	1:B:626:LEU:HG	2.10	0.50
1:D:363:ARG:HB2	1:D:367:GLU:OE1	2.11	0.50
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.46	0.50
1:B:569:TYR:CZ	1:B:629:LYS:HE2	2.47	0.50
1:B:550:MET:HE3	1:B:599:LEU:HD23	1.92	0.50
1:D:315:LEU:CD1	1:D:420:LEU:HD11	2.42	0.49
1:A:436:LEU:HD11	1:B:488:LEU:CD1	2.43	0.49
1:B:333:ASN:HD21	1:B:411:ASP:HA	1.78	0.49
1:B:530[B]:TRP:CZ2	1:D:414:HIS:NE2	2.80	0.49
1:B:548:VAL:HG21	1:B:632:LEU:HD21	1.94	0.49
1:B:358:ARG:HG2	1:B:388:GLN:HG3	1.94	0.49
1:A:633:LEU:HD12	1:A:633:LEU:C	2.33	0.49
1:D:530:TRP:CZ3	1:D:535:PRO:HD3	2.48	0.49
1:B:188:VAL:O	1:B:192:LEU:HG	2.13	0.48
1:B:633:LEU:HD12	1:B:633:LEU:C	2.33	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:352:GLU:HB2	1:A:416:LEU:HB3	1.95	0.48
1:A:441:GLN:O	1:A:445:GLU:HG3	2.13	0.48
1:A:409:CYS:SG	1:A:415:SER:HB3	2.54	0.48
5:A:2191:HOH:O	1:B:482[B]:ARG:HG3	2.12	0.48
1:D:435:ILE:HG13	1:D:497:VAL:HG21	1.95	0.48
1:C:333:ASN:OD1	1:C:411:ASP:HA	2.13	0.48
1:C:420:LEU:C	1:C:420:LEU:HD23	2.33	0.48
1:D:555:ILE:O	1:D:569:TYR:HA	2.14	0.48
1:B:187:ARG:HH11	1:B:187:ARG:HG2	1.79	0.48
1:B:275:LEU:HD12	1:B:275:LEU:N	2.29	0.48
1:D:247:LEU:HA	1:D:250:MET:CE	2.40	0.48
1:D:436:LEU:O	1:D:440[A]:VAL:HG22	2.14	0.48
1:A:275:LEU:HD12	1:A:275:LEU:N	2.29	0.48
1:A:341:TYR:CE1	1:A:374:SER:HB3	2.49	0.48
1:B:568:TYR:CD2	1:B:584:CYS:HB3	2.48	0.48
1:D:359:VAL:O	1:D:386:VAL:HG12	2.14	0.48
1:C:297:ARG:HD3	1:C:328:TYR:CE2	2.49	0.48
1:D:266:ARG:O	1:D:273:GLU:HG2	2.14	0.47
1:D:345:GLU:OE2	1:D:401:ARG:HG2	2.13	0.47
1:A:250:MET:HE1	1:A:298:LEU:HD21	1.95	0.47
1:A:487[A]:ARG:NH1	5:A:2159:HOH:O	2.47	0.47
1:D:386:VAL:O	1:D:386:VAL:HG22	2.14	0.47
1:A:275:LEU:O	1:A:277:PRO:HD3	2.14	0.47
1:D:447:ASN:HD22	1:D:449:GLU:H	1.62	0.47
1:A:297:ARG:HD3	1:A:328:TYR:CE2	2.49	0.47
1:A:418:LEU:C	1:A:418:LEU:HD23	2.34	0.47
1:A:333:ASN:ND2	1:A:411:ASP:HA	2.30	0.47
1:C:527:PRO:O	1:C:528:ILE:HD13	2.14	0.47
1:D:609:GLY:HA2	1:D:619:GLN:OE1	2.14	0.47
1:B:265:ALA:HB1	1:B:272:ARG:HE	1.79	0.47
1:B:633:LEU:O	1:B:633:LEU:HD12	2.15	0.47
1:D:536:VAL:HG12	1:D:536:VAL:O	2.15	0.47
1:C:590:GLN:CD	1:C:590:GLN:H	2.18	0.46
1:D:459:MET:HG3	5:D:2091:HOH:O	2.15	0.46
1:D:361[A]:ARG:HG3	1:D:386:VAL:HB	1.97	0.46
1:D:257:GLN:HE22	1:D:280:ARG:HB2	1.81	0.46
1:D:275:LEU:O	1:D:277:PRO:HD3	2.15	0.46
1:D:298:LEU:HD23	1:D:301:PRO:HG3	1.97	0.46
1:C:197:SER:O	1:C:201:ARG:HG3	2.16	0.46
1:D:553:ASP:HB2	1:D:602:TYR:CE1	2.51	0.46
1:B:374:SER:HB2	1:B:375:PRO:HD2	1.98	0.46
1:D:374:SER:HB2	1:D:375:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:LEU:O	1:A:201:ARG:HD3	2.15	0.46
1:A:536:VAL:HG23	1:A:536:VAL:O	2.15	0.46
1:A:333:ASN:OD1	1:A:411:ASP:HA	2.15	0.45
1:B:531:GLU:O	1:B:532:ALA:HB3	2.16	0.45
1:A:300:CYS:SG	5:A:2084:HOH:O	2.61	0.45
1:C:183:SER:CB	1:C:239:GLN:HB3	2.46	0.45
1:C:506:ILE:HG23	1:C:570:THR:HG22	1.98	0.45
1:D:246:ASP:O	1:D:250:MET:HG3	2.16	0.45
1:A:344:ILE:O	1:A:344:ILE:HD12	2.16	0.45
1:A:182:MET:HE3	1:A:187:ARG:HH11	1.81	0.45
1:B:565:LEU:HB2	1:B:587:ILE:O	2.17	0.45
1:C:250:MET:HE1	1:C:298:LEU:HD21	1.98	0.45
1:C:589:PRO:HD2	1:C:590:GLN:NE2	2.31	0.45
1:D:195:ILE:HB	1:D:201:ARG:HG2	1.99	0.45
1:B:544:THR:HA	1:B:608:VAL:HB	1.98	0.45
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.99	0.45
1:A:501:ARG:HD2	5:A:2149:HOH:O	2.15	0.45
1:B:530[A]:TRP:CZ2	1:D:244:THR:HG21	2.51	0.45
1:D:399:PHE:HA	1:D:400:PRO:HD3	1.79	0.45
1:A:531:GLU:O	1:A:532:ALA:HB3	2.17	0.45
1:A:568:TYR:CD2	1:A:584:CYS:HB3	2.53	0.44
1:B:185:LEU:O	1:B:188:VAL:HG12	2.17	0.44
1:B:341:TYR:CE2	1:B:374:SER:HB3	2.52	0.44
1:B:214:PRO:HA	1:B:215:PRO:HD3	1.87	0.44
1:B:410:GLN:NE2	1:B:410:GLN:HA	2.30	0.44
1:B:542:LEU:HD21	1:B:624:THR:OG1	2.17	0.44
1:C:536:VAL:HG22	1:C:537:ASN:N	2.32	0.44
1:C:640:LEU:HD23	1:C:640:LEU:H	1.81	0.44
1:D:480:LYS:O	1:D:483:VAL:HG12	2.17	0.44
1:D:529:ARG:H	1:D:537:ASN:CB	2.31	0.44
1:C:436:LEU:HD11	1:D:440[A]:VAL:CG1	2.47	0.44
1:B:546:THR:O	1:B:607:ARG:HA	2.18	0.44
1:B:537:ASN:CB	1:D:291:GLN:HE22	2.31	0.44
1:D:528:ILE:HD12	1:D:528:ILE:N	2.32	0.44
1:A:275:LEU:HD22	1:A:294:CYS:SG	2.58	0.44
1:B:432:LEU:HA	1:B:435:ILE:HG22	2.00	0.44
1:C:360:TYR:CE2	1:C:385:PRO:HG3	2.53	0.44
1:A:515:THR:OG1	1:A:518:GLU:HG3	2.17	0.44
1:B:197:SER:O	1:B:201:ARG:HG3	2.18	0.44
1:D:287:TRP:O	1:D:291:GLN:HG3	2.18	0.44
1:D:633:LEU:HD12	1:D:633:LEU:C	2.38	0.43
1:A:436:LEU:O	1:A:440:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:187:ARG:NH1	1:C:187:ARG:HB2	2.34	0.43
1:C:195:ILE:HB	1:C:201:ARG:HG2	1.99	0.43
1:D:297:ARG:HD3	1:D:328:TYR:CE2	2.52	0.43
1:A:315:LEU:CD1	1:A:420:LEU:HD11	2.48	0.43
1:A:404:ILE:HG13	5:A:2125:HOH:O	2.18	0.43
1:A:590:GLN:H	1:A:590:GLN:CD	2.20	0.43
1:C:341:TYR:CZ	1:C:374:SER:HB3	2.54	0.43
1:D:333:ASN:OD1	1:D:411:ASP:HA	2.19	0.43
1:D:418:LEU:C	1:D:418:LEU:HD23	2.39	0.43
1:B:195:ILE:HA	1:B:196:PRO:HD3	1.89	0.43
1:B:451:ARG:HB2	1:B:451:ARG:NH1	2.34	0.43
1:A:386:VAL:HG22	1:A:386:VAL:O	2.18	0.43
1:A:252:ARG:NH1	5:A:2055:HOH:O	2.51	0.43
1:B:435:ILE:HD11	1:B:494:VAL:HA	2.01	0.43
1:C:633:LEU:HD12	1:C:633:LEU:C	2.38	0.43
1:D:344:ILE:CG2	1:D:424:GLN:HB2	2.48	0.43
1:C:503:LYS:HE3	1:C:568:TYR:CZ	2.54	0.43
1:D:363:ARG:HH12	1:D:381:ASP:HB3	1.84	0.43
1:C:345:GLU:OE2	1:C:401:ARG:HG2	2.19	0.42
1:D:231:ARG:NH2	1:D:389:THR:OG1	2.51	0.42
1:D:333:ASN:CG	1:D:411:ASP:HA	2.39	0.42
1:D:531:GLU:O	1:D:532:ALA:HB3	2.19	0.42
1:D:252:ARG:HG3	1:D:252:ARG:HH11	1.83	0.42
1:A:530:TRP:CZ3	1:A:535:PRO:HD3	2.53	0.42
1:A:545:GLU:HG3	1:A:607:ARG:NH2	2.33	0.42
1:A:436:LEU:HD12	1:B:440[B]:VAL:CG2	2.49	0.42
1:D:384:GLU:HA	1:D:385:PRO:HD3	1.93	0.42
1:A:440:VAL:CG2	1:B:436:LEU:HD12	2.48	0.42
1:C:485:VAL:O	1:C:488:LEU:HB2	2.19	0.42
1:B:550:MET:HE3	1:B:599:LEU:CD2	2.48	0.42
1:C:488:LEU:HD11	1:D:436:LEU:HD11	2.00	0.42
1:A:216:ASP:OD2	1:A:220:ARG:NH2	2.51	0.42
1:C:335:GLN:HG3	1:C:407:ALA:O	2.19	0.42
1:C:333:ASN:CG	1:C:411:ASP:HA	2.40	0.42
1:A:542:LEU:N	1:A:542:LEU:HD12	2.35	0.42
1:C:589:PRO:HB2	1:C:590:GLN:HE21	1.85	0.42
1:A:213:MET:HA	1:A:214:PRO:HD3	1.92	0.42
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.84	0.42
1:B:359:VAL:O	1:B:386:VAL:HG12	2.20	0.42
1:B:315:LEU:CD1	1:B:420:LEU:HD11	2.49	0.42
1:D:468:ASP:HB2	5:D:2099:HOH:O	2.20	0.42
1:D:527:PRO:HD2	1:D:639:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:192:LEU:O	1:C:201:ARG:HD3	2.18	0.41
1:D:360:TYR:CE2	1:D:385:PRO:HG3	2.55	0.41
1:A:244:THR:HG21	1:C:530:TRP:CE2	2.55	0.41
1:D:298:LEU:HB3	1:D:327:VAL:HB	2.01	0.41
1:B:542:LEU:H	1:B:542:LEU:CD2	2.28	0.41
1:A:217:HIS:ND1	1:A:221:ARG:HD3	2.35	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.94	0.41
1:D:565:LEU:HB2	1:D:587:ILE:O	2.21	0.41
1:D:546:THR:O	1:D:607:ARG:HA	2.20	0.41
1:A:325:SER:HA	1:A:419:THR:O	2.20	0.41
1:B:266:ARG:HG3	1:B:268:ILE:HD13	2.03	0.41
1:B:553:ASP:HB2	1:B:602:TYR:CE1	2.56	0.41
1:B:549:HIS:C	1:B:632:LEU:HD12	2.42	0.41
1:D:548:VAL:HG21	1:D:632:LEU:HD21	2.03	0.41
1:B:549:HIS:CE1	1:B:633:LEU:HD11	2.56	0.41
1:C:373:SER:HB3	5:C:2096:HOH:O	2.21	0.41
1:A:291:GLN:HE22	1:C:538:VAL:CB	2.34	0.41
1:C:550:MET:HE2	1:C:598:LEU:C	2.41	0.41
1:D:221:ARG:O	1:D:225:ARG:HD2	2.20	0.41
1:C:272:ARG:HG3	1:C:272:ARG:HH11	1.85	0.41
1:C:550:MET:CE	1:C:598:LEU:HB3	2.50	0.41
1:D:214:PRO:HA	1:D:215:PRO:HD3	1.95	0.40
1:D:301:PRO:HB2	1:D:308:VAL:HG11	2.03	0.40
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.86	0.40
1:A:382:LEU:HD22	1:A:404:ILE:HG21	2.04	0.40
1:B:232:ARG:HD3	1:B:237:TYR:CG	2.55	0.40
1:B:287:TRP:HA	1:B:287:TRP:CE3	2.57	0.40
1:C:526:LEU:HG	1:C:528:ILE:HD11	2.03	0.40
1:C:553:ASP:HB2	1:C:602:TYR:CD1	2.56	0.40
1:D:310:GLN:HA	1:D:513:VAL:HG21	2.03	0.40
1:C:429:GLY:O	1:C:433:GLU:HG3	2.22	0.40
1:D:410:GLN:HA	1:D:410:GLN:NE2	2.32	0.40
1:B:267:TYR:CZ	1:B:270:GLY:HA2	2.57	0.40
1:C:440:VAL:CG2	1:D:436:LEU:CD1	2.99	0.40
1:D:223:TRP:CD1	1:D:224:GLU:HG3	2.57	0.40
1:D:568:TYR:CD2	1:D:584:CYS:HB3	2.57	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	454/467 (97%)	446 (98%)	8 (2%)	0	100	100
1	B	456/467 (98%)	442 (97%)	14 (3%)	0	100	100
1	C	458/467 (98%)	450 (98%)	8 (2%)	0	100	100
1	D	458/467 (98%)	443 (97%)	15 (3%)	0	100	100
All	All	1826/1868 (98%)	1781 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/399 (97%)	382 (98%)	6 (2%)	76	83
1	B	382/399 (96%)	369 (97%)	13 (3%)	49	50
1	C	386/399 (97%)	379 (98%)	7 (2%)	71	77
1	D	383/399 (96%)	371 (97%)	12 (3%)	52	54
All	All	1539/1596 (96%)	1501 (98%)	38 (2%)	64	64

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	232	ARG
1	A	280	ARG
1	A	468	ASP
1	A	590	GLN

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Mol	Chain	Res	Type
1	A	603	PRO
1	B	187	ARG
1	B	232	ARG
1	B	233	GLN
1	B	280	ARG
1	B	410	GLN
1	B	420	LEU
1	B	435	ILE
1	B	451	ARG
1	B	530[A]	TRP
1	B	530[B]	TRP
1	B	550	MET
1	B	590	GLN
1	B	607	ARG
1	C	232	ARG
1	C	255	GLU
1	C	410	GLN
1	C	517[A]	ARG
1	C	517[B]	ARG
1	C	534	GLU
1	C	603	PRO
1	D	187[A]	ARG
1	D	187[B]	ARG
1	D	194	ARG
1	D	232	ARG
1	D	410	GLN
1	D	435	ILE
1	D	440[A]	VAL
1	D	440[B]	VAL
1	D	447	ASN
1	D	468	ASP
1	D	580	GLU
1	D	636	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	257	GLN
1	A	291	GLN
1	A	410	GLN
1	A	500	GLN

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Mol	Chain	Res	Type
1	A	537	ASN
1	B	257	GLN
1	B	326	ASN
1	B	410	GLN
1	B	424	GLN
1	B	590	GLN
1	C	318	GLN
1	C	414	HIS
1	C	424	GLN
1	C	590	GLN
1	D	257	GLN
1	D	291	GLN
1	D	379	GLN
1	D	406	GLN
1	D	410	GLN
1	D	447	ASN
1	D	500	GLN
1	D	590	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, 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	456/467 (97%)	-0.14	1 (0%) 93 96	22, 34, 58, 78	1 (0%)
1	B	456/467 (97%)	-0.01	7 (1%) 70 76	22, 41, 86, 100	3 (0%)
1	C	458/467 (98%)	-0.06	9 (1%) 62 67	23, 36, 63, 93	2 (0%)
1	D	459/467 (98%)	-0.04	8 (1%) 67 73	24, 46, 80, 100	0
All	All	1829/1868 (97%)	-0.06	25 (1%) 68 77	22, 39, 74, 100	6 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	530[A]	TRP	9.0
1	C	528	ILE	5.7
1	C	640	LEU	5.2
1	B	536	VAL	4.7
1	D	538	VAL	4.6
1	C	530	TRP	4.4
1	C	532	ALA	3.5
1	B	532	ALA	3.4
1	A	639	ALA	3.2
1	B	588	TYR	2.9
1	C	639	ALA	2.8
1	C	537	ASN	2.8
1	C	468[A]	ASP	2.7
1	D	641	ASN	2.7
1	D	540	ALA	2.6
1	C	535	PRO	2.5
1	B	617	GLU	2.4
1	D	537	ASN	2.4
1	B	614	ASP	2.3
1	D	268	ILE	2.3
1	D	636	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	536	VAL	2.1
1	B	520	ALA	2.1
1	D	361[A]	ARG	2.0
1	D	562	GLY	2.0

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	A	901	1/1	0.20	22.56	18,18,18,18	0
2	MN	B	901	1/1	0.18	12.26	18,18,18,18	0
4	EDO	D	903	4/4	0.18	11.98	50,51,52,52	0
2	MN	C	901	1/1	0.20	9.06	20,20,20,20	0
2	MN	D	901	1/1	0.18	7.13	28,28,28,28	0
4	EDO	B	903	4/4	0.15	4.83	32,37,38,42	0
4	EDO	C	903	4/4	0.12	2.49	34,35,35,37	0
3	OGA	D	902	10/10	0.12	0.90	52,54,57,57	0
4	EDO	A	903	4/4	0.10	0.62	31,35,36,37	0
3	OGA	B	902	10/10	0.10	-0.07	37,43,47,48	0
3	OGA	A	902	10/10	0.10	-0.85	36,41,43,45	0
3	OGA	C	902	10/10	0.09	-0.90	38,40,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.