



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2018 – 06:21 AM EST

PDB ID : 4CCJ
Title : 60S ribosomal protein L8 histidine hydroxylase (NO66) in apo form
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 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

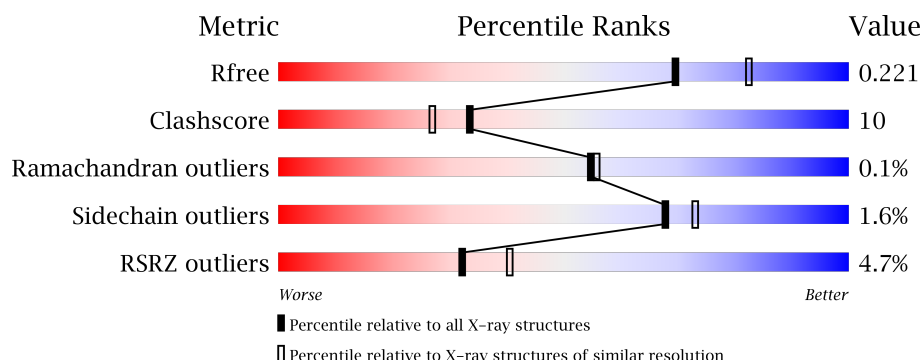
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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. 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> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
1	B	467	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
1	C	467	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>••</div> </div> </div>
1	D	467	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	1640	-	-	-	X
2	EDO	C	1640	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15725 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	9	0
			3718	2365	658	678	17			
1	B	458	Total	C	N	O	S	0	7	0
			3698	2353	656	672	17			
1	C	458	Total	C	N	O	S	0	5	0
			3690	2351	650	673	16			
1	D	457	Total	C	N	O	S	0	4	0
			3664	2334	647	667	16			

There are 36 discrepancies between the modelled and reference sequences:

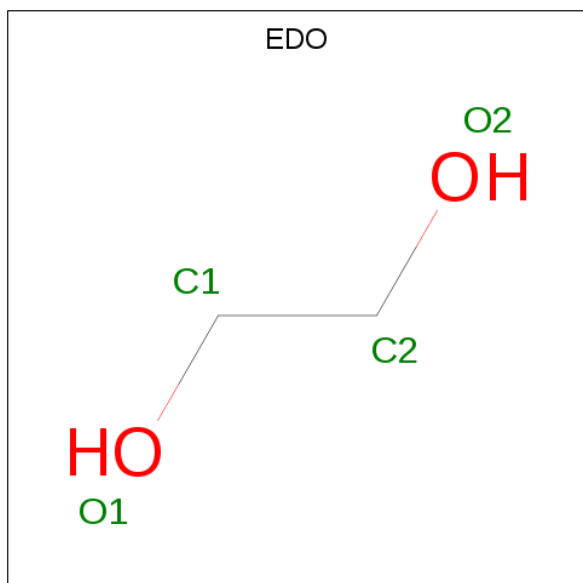
Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	expression tag	UNP Q9H6W3
A	642	ALA	-	expression tag	UNP Q9H6W3
A	643	GLU	-	expression tag	UNP Q9H6W3
A	644	ASN	-	expression tag	UNP Q9H6W3
A	645	LEU	-	expression tag	UNP Q9H6W3
A	646	TYR	-	expression tag	UNP Q9H6W3
A	647	PHE	-	expression tag	UNP Q9H6W3
A	648	GLN	-	expression tag	UNP Q9H6W3
A	364	ALA	VAL	engineered mutation	UNP Q9H6W3
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
C	182	MET	-	expression tag	UNP Q9H6W3
C	642	ALA	-	expression tag	UNP Q9H6W3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	643	GLU	-	expression tag	UNP Q9H6W3
C	644	ASN	-	expression tag	UNP Q9H6W3
C	645	LEU	-	expression tag	UNP Q9H6W3
C	646	TYR	-	expression tag	UNP Q9H6W3
C	647	PHE	-	expression tag	UNP Q9H6W3
C	648	GLN	-	expression tag	UNP Q9H6W3
C	364	ALA	VAL	engineered mutation	UNP Q9H6W3
D	182	MET	-	expression tag	UNP Q9H6W3
D	642	ALA	-	expression tag	UNP Q9H6W3
D	643	GLU	-	expression tag	UNP Q9H6W3
D	644	ASN	-	expression tag	UNP Q9H6W3
D	645	LEU	-	expression tag	UNP Q9H6W3
D	646	TYR	-	expression tag	UNP Q9H6W3
D	647	PHE	-	expression tag	UNP Q9H6W3
D	648	GLN	-	expression tag	UNP Q9H6W3
D	364	ALA	VAL	engineered mutation	UNP Q9H6W3

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



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

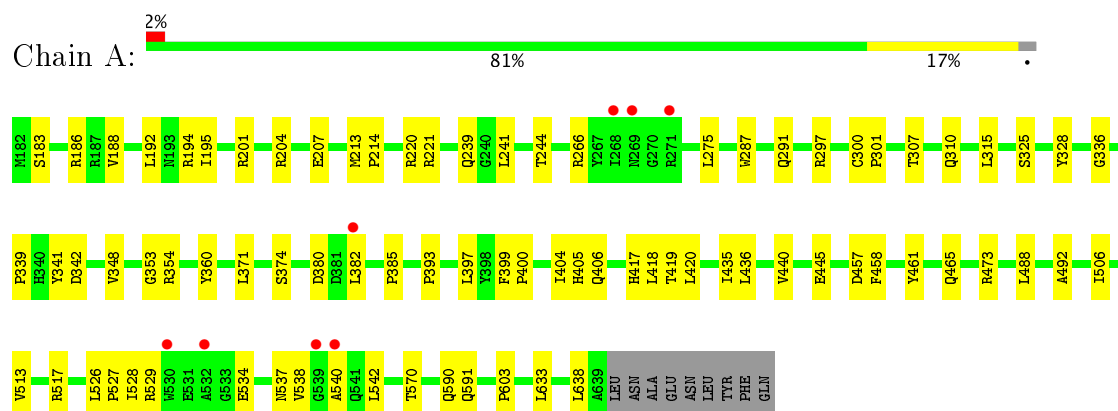
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	329	Total 329	O 329	0	0
3	B	288	Total 288	O 288	0	0
3	C	173	Total 173	O 173	0	0
3	D	153	Total 153	O 153	0	0

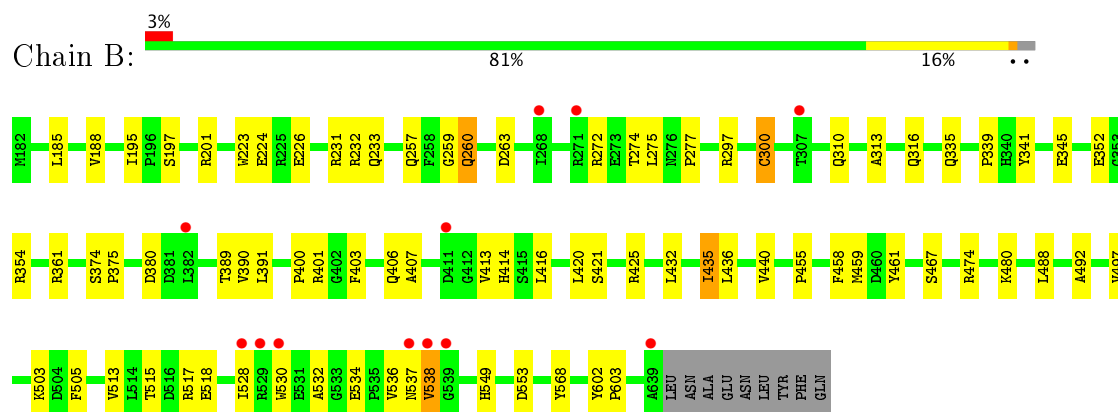
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

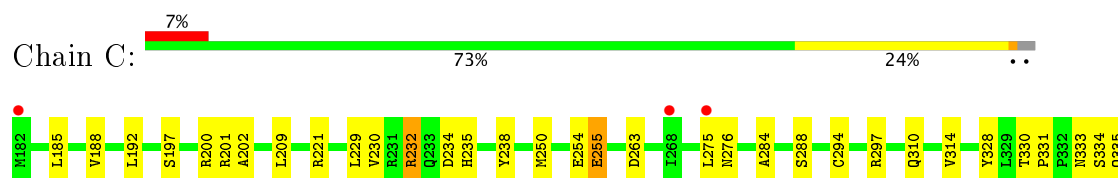
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

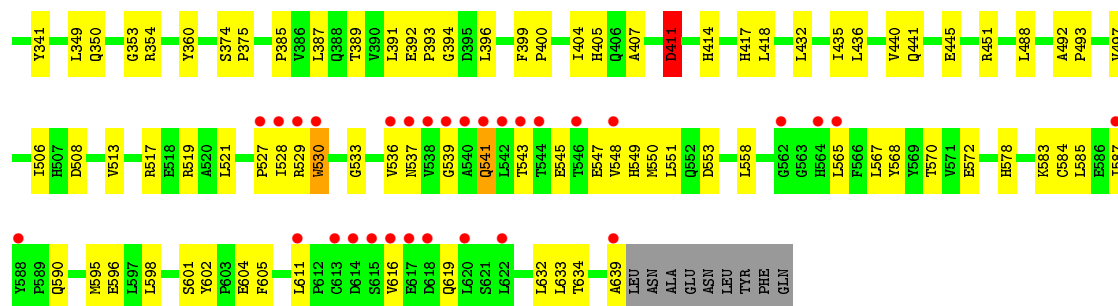


• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

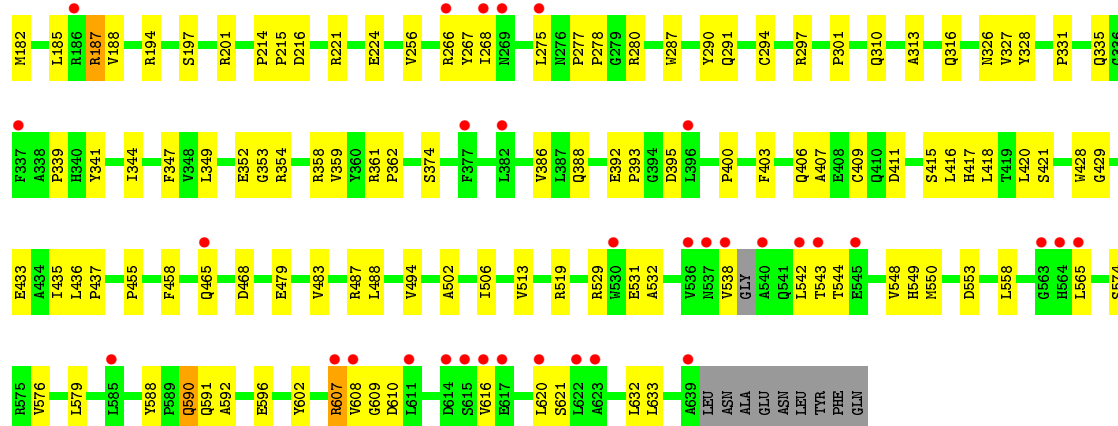
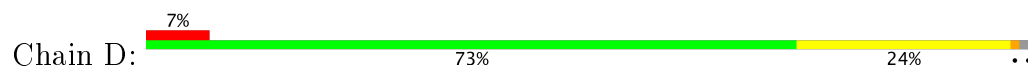


• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.44Å 81.56Å 151.96Å 90.00° 94.66° 90.00°	Depositor
Resolution (Å)	63.72 – 2.15 63.72 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.1 (63.72-2.15) 94.9 (63.72-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.16Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.202 , 0.210 0.217 , 0.221	Depositor DCC
R_{free} test set	6443 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15725	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/3840	0.62	0/5222
1	B	0.40	0/3814	0.64	1/5190 (0.0%)
1	C	0.36	0/3802	0.62	3/5174 (0.1%)
1	D	0.36	0/3770	0.57	1/5129 (0.0%)
All	All	0.37	0/15226	0.61	5/20715 (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	C	0	4
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	611	LEU	CB-CA-C	5.58	120.81	110.20
1	D	411	ASP	N-CA-C	5.56	126.00	111.00
1	C	234	ASP	N-CA-CB	-5.51	100.67	110.60
1	B	259	GLY	N-CA-C	5.38	126.54	113.10
1	C	411	ASP	CB-CA-C	-5.10	100.21	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	517[A]	ARG	Mainchain
1	C	517[B]	ARG	Mainchain
1	C	530[A]	TRP	Mainchain
1	C	530[B]	TRP	Mainchain
1	D	187[A]	ARG	Mainchain
1	D	187[B]	ARG	Mainchain

5.2 Too-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 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	3718	0	3652	61	0
1	B	3698	0	3637	67	0
1	C	3690	0	3605	92	0
1	D	3664	0	3579	90	0
2	B	4	0	6	1	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
3	A	329	0	0	4	0
3	B	288	0	0	5	0
3	C	173	0	0	1	0
3	D	153	0	0	1	0
All	All	15725	0	14491	285	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 10.

All (285) 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:272:ARG:HH12	1:B:274:THR:HG22	1.20	1.01
1:B:455:PRO:HG2	1:B:458:PHE:HB3	1.43	1.01
1:C:263:ASP:HA	1:C:276:ASN:HD21	1.36	0.89
1:A:291:GLN:HE21	1:B:538:VAL:HG11	1.38	0.87
1:C:549:HIS:O	1:C:632:LEU:HD12	1.75	0.87
1:B:272:ARG:NH1	1:B:274:THR:HG22	1.93	0.83
1:A:300[B]:CYS:SG	3:A:2105:HOH:O	2.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300[B]:CYS:SG	3:B:2084:HOH:O	2.33	0.82
1:D:455:PRO:HG2	1:D:458:PHE:HB3	1.62	0.81
1:B:257:GLN:HB2	1:B:260:GLN:HG2	1.63	0.80
1:B:528:ILE:HD13	1:B:538:VAL:HG13	1.63	0.80
1:C:547:GLU:HB3	1:C:605:PHE:HB3	1.68	0.75
1:B:354:ARG:HG2	1:B:390:VAL:HG12	1.69	0.74
1:A:436:LEU:HD13	1:C:436:LEU:HB3	1.69	0.74
1:D:361:ARG:HG2	1:D:362:PRO:HD2	1.70	0.73
1:B:436:LEU:HD13	1:D:436:LEU:HB3	1.70	0.71
1:A:436:LEU:HD11	1:C:488:LEU:HD13	1.73	0.71
1:D:297[A]:ARG:NH1	1:D:326:ASN:OD1	2.24	0.70
1:B:354:ARG:HG2	1:B:390:VAL:CG1	2.21	0.70
1:D:487:ARG:HD2	3:D:2115:HOH:O	1.90	0.70
1:C:587:ILE:HD13	1:C:595:MET:HG2	1.74	0.69
3:B:2212:HOH:O	1:D:465:GLN:HG3	1.92	0.69
1:A:529:ARG:H	1:A:537:ASN:CB	2.06	0.68
1:C:529:ARG:O	1:C:536:VAL:HG22	1.93	0.67
1:A:457:ASP:OD2	1:A:473[B]:ARG:NH2	2.29	0.66
1:B:339:PRO:HG3	1:B:406:GLN:OE1	1.94	0.66
1:C:633:LEU:HD12	1:C:633:LEU:O	1.97	0.65
1:C:435:ILE:HG12	1:C:492:ALA:HB1	1.77	0.64
1:D:358:ARG:HG2	1:D:388:GLN:HG3	1.79	0.64
1:D:574:SER:OG	1:D:576:VAL:HG12	1.97	0.64
1:D:341:TYR:CZ	1:D:374:SER:HB3	2.33	0.64
1:D:297[A]:ARG:NH1	1:D:328:TYR:OH	2.32	0.63
1:D:588:TYR:HB2	1:D:591:GLN:NE2	2.13	0.63
1:C:229:LEU:HD22	1:C:389:THR:HG21	1.80	0.63
1:D:335:GLN:HG3	1:D:407:ALA:O	1.99	0.62
1:D:349:LEU:N	1:D:349:LEU:HD12	2.14	0.62
1:B:354:ARG:HG3	1:B:391:LEU:O	1.99	0.62
1:D:301:PRO:HG2	1:D:327:VAL:HG23	1.81	0.61
1:B:459:MET:HG3	3:B:2188:HOH:O	2.00	0.61
1:A:436:LEU:HD12	1:C:440:VAL:CG2	2.30	0.61
1:B:352:GLU:HB2	1:B:416:LEU:HB3	1.83	0.61
1:D:352:GLU:HB2	1:D:416:LEU:HB3	1.83	0.60
1:C:310:GLN:HA	1:C:513:VAL:HG21	1.84	0.60
1:B:532:ALA:O	1:B:534:GLU:HG2	2.02	0.60
1:D:287:TRP:O	1:D:291:GLN:HG3	2.01	0.59
1:D:310:GLN:HA	1:D:513:VAL:HG11	1.84	0.59
1:D:313:ALA:O	1:D:316:GLN:HG2	2.02	0.59
1:A:436:LEU:O	1:A:440:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ILE:HD12	1:C:497:VAL:HG21	1.84	0.59
1:D:182:MET:O	1:D:187[A]:ARG:NH1	2.36	0.59
1:D:543:THR:O	1:D:608:VAL:HG11	2.03	0.59
1:A:542:LEU:HD12	1:A:542:LEU:H	1.67	0.58
1:C:255[A]:GLU:HG3	3:C:2031:HOH:O	2.02	0.58
1:B:436:LEU:HD11	1:D:488:LEU:HD13	1.84	0.58
1:D:354:ARG:HG3	1:D:354:ARG:HH11	1.69	0.58
1:D:592:ALA:O	1:D:596:GLU:HG3	2.04	0.58
1:C:558:LEU:HD11	1:C:565:LEU:HG	1.84	0.58
1:B:480:LYS:HD3	1:D:428:TRP:CZ2	2.40	0.57
1:D:620:LEU:HD12	1:D:621:SER:N	2.20	0.57
1:B:425[A]:ARG:HD3	3:B:2119:HOH:O	2.04	0.57
1:D:267:TYR:C	1:D:268:ILE:HD12	2.24	0.57
1:A:371:LEU:HD21	1:C:451:ARG:HG3	1.86	0.56
1:A:360:TYR:CE2	1:A:385:PRO:HG3	2.41	0.56
1:A:183:SER:OG	1:A:186:ARG:HG3	2.05	0.56
1:B:335:GLN:HG3	1:B:407:ALA:O	2.05	0.56
1:A:436:LEU:HD11	1:C:488:LEU:CD1	2.36	0.56
1:A:195:ILE:HB	1:A:201:ARG:HG2	1.87	0.56
1:D:529:ARG:H	1:D:538:VAL:C	2.09	0.56
1:B:400:PRO:HG2	1:B:403:PHE:CE1	2.40	0.56
1:C:333:ASN:OD1	1:C:411:ASP:HA	2.05	0.55
1:A:517:ARG:NH1	3:A:2010:HOH:O	2.38	0.55
1:C:341:TYR:CZ	1:C:374:SER:HB3	2.43	0.54
1:A:440:VAL:CG2	1:C:436:LEU:HD12	2.38	0.54
1:A:488:LEU:CD1	1:C:436:LEU:HD11	2.39	0.53
1:C:548:VAL:HG12	1:C:634:THR:HG22	1.90	0.53
1:C:202:ALA:HA	1:C:314:VAL:HG12	1.90	0.53
1:B:420:LEU:HD23	1:B:421:SER:N	2.24	0.53
1:B:536:VAL:O	1:B:537:ASN:HB2	2.08	0.53
1:B:432:LEU:O	1:B:435:ILE:HG22	2.08	0.53
1:B:528:ILE:CD1	1:B:538:VAL:HG13	2.35	0.53
1:C:616:VAL:HA	1:C:619:GLN:NE2	2.22	0.53
1:D:607:ARG:HG2	1:D:609:GLY:H	1.74	0.53
1:C:568:TYR:CD2	1:C:584:CYS:HB3	2.43	0.53
1:A:204:ARG:O	1:A:207:GLU:HG2	2.09	0.53
1:B:231:ARG:NH2	1:B:389[B]:THR:OG1	2.42	0.53
1:A:244:THR:HG21	1:B:530:TRP:CE2	2.43	0.53
1:D:347:PHE:HB2	1:D:420:LEU:HB3	1.91	0.53
1:C:548:VAL:HG21	1:C:632:LEU:HD21	1.90	0.53
1:D:607:ARG:HD2	1:D:610:ASP:CG	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ARG:HD3	1:C:394:GLY:O	2.09	0.52
1:B:435:ILE:HD12	1:B:497:VAL:HG21	1.89	0.52
1:A:440:VAL:HG21	1:C:436:LEU:HD12	1.92	0.52
1:C:235:HIS:HA	1:C:393:PRO:O	2.08	0.52
1:B:517:ARG:NH1	3:B:2010:HOH:O	2.43	0.52
1:A:188:VAL:O	1:A:192:LEU:HG	2.09	0.52
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.91	0.52
1:C:553:ASP:HB2	1:C:602:TYR:CE2	2.45	0.52
1:D:576:VAL:HG13	1:D:579:LEU:HB2	1.92	0.52
1:A:275:LEU:N	1:A:275:LEU:HD22	2.25	0.52
1:D:185:LEU:O	1:D:188:VAL:HG12	2.09	0.52
1:D:436:LEU:HB2	1:D:437:PRO:HD3	1.91	0.51
1:A:287:TRP:HA	1:A:287:TRP:CE3	2.46	0.51
1:B:436:LEU:CD1	1:D:436:LEU:HB3	2.39	0.51
1:A:528:ILE:N	1:A:528:ILE:HD12	2.25	0.51
1:C:590:GLN:CD	1:C:590:GLN:H	2.14	0.51
1:C:353:GLY:O	1:C:393:PRO:HD3	2.11	0.51
1:C:506:ILE:HG23	1:C:570:THR:CG2	2.41	0.51
1:C:506:ILE:HG23	1:C:570:THR:HG22	1.92	0.51
1:A:633:LEU:HD12	1:A:633:LEU:C	2.31	0.51
1:B:226:GLU:OE2	1:B:361[A]:ARG:NH2	2.44	0.51
1:D:275:LEU:N	1:D:275:LEU:HD12	2.25	0.51
1:D:400:PRO:HG2	1:D:403:PHE:CE1	2.46	0.51
1:A:220:ARG:HG2	1:A:221:ARG:NE	2.26	0.50
1:C:441:GLN:O	1:C:445:GLU:HG3	2.11	0.50
1:C:572:GLU:HB2	1:C:583:LYS:HD2	1.92	0.50
1:B:505:PHE:HB2	2:B:1640:EDO:H22	1.94	0.50
1:A:241:LEU:HD12	1:A:307:THR:HG22	1.93	0.50
1:B:272:ARG:HH12	1:B:274:THR:CG2	2.07	0.50
1:B:374:SER:HB2	1:B:375:PRO:HD2	1.93	0.50
1:A:339:PRO:HB3	1:A:406:GLN:HB3	1.92	0.50
1:C:197:SER:O	1:C:201:ARG:HG3	2.12	0.50
1:B:275:LEU:O	1:B:277:PRO:HD3	2.12	0.50
1:C:297:ARG:HD3	1:C:328:TYR:CE2	2.47	0.49
1:C:549:HIS:C	1:C:632:LEU:HD12	2.32	0.49
1:D:479:GLU:O	1:D:483:VAL:HG23	2.10	0.49
1:A:354:ARG:HG3	1:A:354:ARG:HH11	1.76	0.49
1:B:263:ASP:OD2	1:B:297[B]:ARG:NH1	2.45	0.49
1:D:290:TYR:CD1	1:D:331:PRO:HG3	2.47	0.49
1:B:515:THR:OG1	1:B:518:GLU:HG3	2.12	0.49
1:C:275:LEU:N	1:C:275:LEU:HD22	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:O	1:B:316:GLN:HG2	2.13	0.49
1:A:342:ASP:OD2	1:A:405:HIS:HE1	1.95	0.49
1:D:359:VAL:O	1:D:386:VAL:HG12	2.13	0.49
1:B:435:ILE:HG12	1:B:492:ALA:HB1	1.94	0.49
1:C:527:PRO:HD2	1:C:639:ALA:HB3	1.95	0.49
1:C:587:ILE:CD1	1:C:595:MET:HG2	2.41	0.49
1:D:429:GLY:O	1:D:433:GLU:HG3	2.13	0.49
1:A:382:LEU:HD22	1:A:404:ILE:HG21	1.95	0.48
1:A:488:LEU:HD11	1:C:436:LEU:HD11	1.95	0.48
1:B:185:LEU:O	1:B:188:VAL:HG12	2.13	0.48
1:B:341:TYR:CZ	1:B:374:SER:HB3	2.48	0.48
1:B:420:LEU:HD23	1:B:420:LEU:C	2.34	0.48
1:C:349:LEU:N	1:C:349:LEU:HD12	2.29	0.48
1:C:530[B]:TRP:CZ2	1:C:533:GLY:HA2	2.48	0.48
1:A:404:ILE:HG13	3:A:2151:HOH:O	2.13	0.48
1:A:542:LEU:N	1:A:542:LEU:HD12	2.28	0.48
1:C:551:LEU:HD12	1:C:633:LEU:HD23	1.96	0.48
1:A:241:LEU:HA	1:A:307:THR:HG21	1.96	0.48
1:B:503:LYS:HD2	1:B:568:TYR:CZ	2.48	0.48
1:D:633:LEU:C	1:D:633:LEU:HD12	2.34	0.48
1:A:540:ALA:HB1	1:A:638:LEU:HB3	1.96	0.48
1:B:223:TRP:CD1	1:B:224:GLU:HG3	2.49	0.48
1:D:328:TYR:HB2	1:D:417:HIS:CE1	2.48	0.48
1:C:335:GLN:HG3	1:C:407:ALA:O	2.14	0.47
1:D:513:VAL:O	1:D:513:VAL:HG23	2.14	0.47
1:B:413:VAL:HG22	1:B:414:HIS:N	2.29	0.47
1:A:291:GLN:NE2	1:B:538:VAL:HG11	2.17	0.47
1:C:418:LEU:C	1:C:418:LEU:HD23	2.34	0.47
1:A:297:ARG:HD3	1:A:328:TYR:CE2	2.49	0.47
1:C:435:ILE:HD12	1:C:497:VAL:CG2	2.44	0.47
1:D:418:LEU:C	1:D:418:LEU:HD23	2.35	0.47
1:A:341:TYR:CZ	1:A:374:SER:HB3	2.50	0.47
1:D:290:TYR:CE1	1:D:331:PRO:HG3	2.50	0.47
1:D:549:HIS:C	1:D:632:LEU:HD12	2.35	0.47
1:D:558:LEU:HD11	1:D:565:LEU:HB3	1.97	0.47
1:B:553:ASP:HB2	1:B:602:TYR:CE1	2.50	0.47
1:C:209:LEU:C	1:C:232:ARG:HH22	2.19	0.47
1:C:188:VAL:O	1:C:192:LEU:HG	2.14	0.46
1:A:540:ALA:CB	1:A:638:LEU:HB3	2.45	0.46
1:D:268:ILE:N	1:D:268:ILE:HD12	2.31	0.46
1:B:488:LEU:CD1	1:D:436:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:HIS:O	1:D:632:LEU:HD12	2.15	0.46
1:A:310:GLN:HA	1:A:513:VAL:HG21	1.96	0.46
1:B:345:GLU:OE1	1:B:400:PRO:HB3	2.15	0.46
1:D:590:GLN:HE21	1:D:590:GLN:HB2	1.60	0.46
1:A:435:ILE:CD1	1:A:492:ALA:HB1	2.46	0.46
1:C:567:LEU:HB2	1:C:587:ILE:HD11	1.96	0.46
1:D:266:ARG:HB3	1:D:268:ILE:CD1	2.46	0.46
1:B:458:PHE:HA	1:B:461:TYR:CZ	2.50	0.46
1:C:328:TYR:HB2	1:C:417:HIS:CE1	2.51	0.46
1:D:339:PRO:HB3	1:D:406:GLN:HB3	1.97	0.46
1:B:197:SER:O	1:B:201:ARG:HG3	2.16	0.46
1:D:553:ASP:HB2	1:D:602:TYR:CE1	2.50	0.46
1:C:530[A]:TRP:CZ2	1:C:533:GLY:HA2	2.51	0.46
1:D:544:THR:HA	1:D:608:VAL:HG13	1.98	0.46
1:D:341:TYR:CE2	1:D:374:SER:HB3	2.51	0.45
1:A:315:LEU:HD13	1:A:420:LEU:HD11	1.98	0.45
1:A:534:GLU:OE2	1:B:414:HIS:HD2	1.99	0.45
1:C:360:TYR:CE2	1:C:385:PRO:HG3	2.50	0.45
1:C:374:SER:HB2	1:C:375:PRO:HD2	1.99	0.45
1:A:418:LEU:HD23	1:A:418:LEU:C	2.37	0.45
1:B:195:ILE:HB	1:B:201:ARG:HG2	1.98	0.45
1:C:616:VAL:HA	1:C:619:GLN:HE21	1.82	0.45
1:B:440:VAL:CG2	1:D:436:LEU:CD1	2.95	0.45
1:B:272:ARG:NH1	1:B:274:THR:CG2	2.72	0.45
1:B:345:GLU:OE2	1:B:401:ARG:HG2	2.17	0.45
1:A:325:SER:HA	1:A:419:THR:O	2.18	0.44
1:B:440:VAL:CG2	1:D:436:LEU:HD12	2.47	0.44
1:D:420:LEU:HD23	1:D:421:SER:N	2.32	0.44
1:A:458:PHE:HA	1:A:461:TYR:CZ	2.52	0.44
1:D:275:LEU:O	1:D:277:PRO:HD3	2.17	0.44
1:D:519:ARG:NH1	1:D:519:ARG:HB2	2.31	0.44
1:D:548:VAL:HB	1:D:632:LEU:HD11	2.00	0.44
1:C:585:LEU:C	1:C:585:LEU:HD12	2.38	0.44
1:D:197:SER:O	1:D:201:ARG:HG3	2.18	0.44
1:D:361:ARG:HG2	1:D:362:PRO:CD	2.43	0.44
3:A:2159:HOH:O	1:C:451:ARG:HG2	2.18	0.44
1:C:354[B]:ARG:HA	1:C:391:LEU:O	2.18	0.44
1:D:266:ARG:HG2	1:D:294:CYS:HA	2.00	0.44
1:C:548:VAL:CG1	1:C:634:THR:HG22	2.48	0.44
1:B:440:VAL:HG21	1:D:436:LEU:HD12	2.00	0.44
1:D:531:GLU:O	1:D:532:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:VAL:O	1:D:620:LEU:HG	2.17	0.44
1:C:221:ARG:HG3	1:C:221:ARG:HH11	1.82	0.43
1:C:508:ASP:OD1	1:C:578:HIS:NE2	2.49	0.43
1:D:301:PRO:CG	1:D:327:VAL:HG23	2.48	0.43
1:B:435:ILE:HD12	1:B:497:VAL:CG2	2.49	0.43
1:D:353:GLY:O	1:D:393:PRO:HD3	2.17	0.43
1:C:399:PHE:HA	1:C:400:PRO:HD3	1.84	0.43
1:B:275:LEU:HD12	1:B:275:LEU:N	2.33	0.43
1:B:432:LEU:HA	1:B:435:ILE:HG22	2.00	0.43
1:C:250:MET:O	1:C:254:GLU:HB2	2.18	0.43
1:C:432:LEU:HA	1:C:435:ILE:HG22	2.00	0.43
1:C:548:VAL:HG12	1:C:634:THR:HA	1.99	0.43
1:D:266:ARG:HB3	1:D:268:ILE:HD13	2.00	0.43
1:B:528:ILE:HD12	1:B:536:VAL:O	2.19	0.43
1:C:435:ILE:HD11	1:C:493:PRO:C	2.39	0.43
1:A:192:LEU:O	1:A:201:ARG:HD3	2.19	0.43
1:D:392:GLU:HG2	1:D:395:ASP:OD2	2.19	0.43
1:B:436:LEU:HD11	1:D:488:LEU:CD1	2.47	0.42
1:C:519:ARG:HH11	1:C:519:ARG:HG3	1.84	0.42
1:A:353:GLY:O	1:A:393:PRO:HD3	2.20	0.42
1:D:362:PRO:HD3	1:D:403:PHE:CE1	2.54	0.42
1:A:301:PRO:HG2	1:A:325:SER:OG	2.18	0.42
1:C:354[A]:ARG:HE	1:C:392:GLU:HG2	1.84	0.42
1:D:386:VAL:O	1:D:386:VAL:HG22	2.18	0.42
1:D:550:MET:CE	1:D:632:LEU:HD13	2.49	0.42
1:B:467:SER:HA	1:B:474:ARG:NH2	2.34	0.42
1:D:256:VAL:O	1:D:280:ARG:HG3	2.20	0.42
1:C:185:LEU:O	1:C:188:VAL:HG12	2.20	0.42
1:C:539:GLY:O	1:C:541:GLN:HG3	2.20	0.42
1:D:344:ILE:HD12	1:D:344:ILE:O	2.19	0.42
1:D:550:MET:HE2	1:D:632:LEU:HD13	2.02	0.42
1:D:409:CYS:SG	1:D:415:SER:HB3	2.60	0.42
1:A:506:ILE:HG23	1:A:570:THR:HG22	2.00	0.42
1:C:331:PRO:HG2	1:C:334:SER:OG	2.19	0.42
1:A:348:VAL:HB	1:A:397:LEU:HB3	2.00	0.42
1:C:404:ILE:HG22	1:C:405:HIS:N	2.35	0.41
1:C:435:ILE:CG1	1:C:492:ALA:HB1	2.45	0.41
1:A:244:THR:HG21	1:B:530:TRP:CD2	2.55	0.41
1:C:528:ILE:HG12	1:C:537:ASN:O	2.20	0.41
1:C:530[B]:TRP:CE2	1:C:533:GLY:HA2	2.55	0.41
1:C:230:VAL:HB	1:C:396:LEU:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:LEU:HD21	1:C:389:THR:HG22	2.01	0.41
1:D:277:PRO:HA	1:D:278:PRO:HD3	1.95	0.41
1:D:435:ILE:HD11	1:D:494:VAL:HA	2.02	0.41
1:D:502:ALA:O	1:D:506:ILE:HG12	2.20	0.41
1:D:588:TYR:HB2	1:D:591:GLN:HE21	1.84	0.41
1:A:213:MET:HA	1:A:214:PRO:HD3	1.94	0.41
1:A:465[B]:GLN:HE21	1:C:596:GLU:HG2	1.84	0.41
1:A:436:LEU:HD12	1:C:440:VAL:HG23	2.02	0.41
1:B:233:GLN:NE2	1:B:233:GLN:HA	2.36	0.41
1:C:284:ALA:O	1:C:288:SER:HB2	2.19	0.41
1:C:330:THR:O	1:C:414:HIS:HB2	2.21	0.41
1:C:530[A]:TRP:CE2	1:C:533:GLY:HA2	2.56	0.41
1:D:214:PRO:HA	1:D:215:PRO:HD3	1.85	0.41
1:D:542:LEU:HD12	1:D:542:LEU:N	2.36	0.41
1:A:328:TYR:HB2	1:A:417:HIS:CE1	2.55	0.41
1:A:526:LEU:HA	1:A:527:PRO:HD3	1.94	0.41
1:C:354[A]:ARG:HA	1:C:391:LEU:O	2.20	0.41
1:C:601:SER:O	1:C:604:GLU:HG2	2.20	0.41
1:A:266:ARG:HA	1:A:336:GLY:HA2	2.02	0.41
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.78	0.41
1:B:354:ARG:CG	1:B:390:VAL:HG12	2.45	0.41
1:C:275:LEU:HD23	1:C:294:CYS:SG	2.61	0.41
1:C:238:TYR:CD2	1:C:350:GLN:O	2.74	0.41
1:C:550:MET:CE	1:C:598:LEU:HB3	2.51	0.41
1:D:420:LEU:C	1:D:420:LEU:HD23	2.41	0.40
1:C:200:ARG:HH11	1:C:200:ARG:HG2	1.86	0.40
1:D:607:ARG:HD2	1:D:610:ASP:OD2	2.21	0.40
1:D:224:GLU:HA	1:D:400:PRO:HB3	2.04	0.40
1:C:543:THR:HG23	1:C:545:GLU:H	1.86	0.40
1:D:607:ARG:HD3	1:D:609:GLY:HA3	2.02	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	465/467 (100%)	459 (99%)	5 (1%)	1 (0%)	51	50
1	B	463/467 (99%)	450 (97%)	13 (3%)	0	100	100
1	C	461/467 (99%)	444 (96%)	17 (4%)	0	100	100
1	D	457/467 (98%)	443 (97%)	14 (3%)	0	100	100
All	All	1846/1868 (99%)	1796 (97%)	49 (3%)	1 (0%)	55	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	VAL

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	396/399 (99%)	389 (98%)	7 (2%)	64	68
1	B	394/399 (99%)	385 (98%)	9 (2%)	56	59
1	C	390/399 (98%)	385 (99%)	5 (1%)	73	79
1	D	386/399 (97%)	380 (98%)	6 (2%)	68	73
All	All	1566/1596 (98%)	1539 (98%)	27 (2%)	68	71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194[A]	ARG
1	A	194[B]	ARG
1	A	239	GLN
1	A	380	ASP
1	A	590	GLN
1	A	591	GLN
1	A	603	PRO

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Mol	Chain	Res	Type
1	B	232	ARG
1	B	260	GLN
1	B	300[A]	CYS
1	B	300[B]	CYS
1	B	380	ASP
1	B	435	ILE
1	B	538	VAL
1	B	549	HIS
1	B	603	PRO
1	C	232	ARG
1	C	255[A]	GLU
1	C	255[B]	GLU
1	C	411	ASP
1	C	541	GLN
1	D	194	ARG
1	D	216	ASP
1	D	221	ARG
1	D	468	ASP
1	D	590	GLN
1	D	607	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	A	405	HIS
1	B	233	GLN
1	B	239	GLN
1	B	405	HIS
1	B	441	GLN
1	C	441	GLN
1	C	590	GLN
1	C	619	GLN
1	D	233	GLN
1	D	260	GLN
1	D	335	GLN
1	D	405	HIS
1	D	417	HIS
1	D	537	ASN
1	D	590	GLN
1	D	591	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	EDO	B	1640	-	3,3,3	0.54	0	2,2,2	0.27	0
2	EDO	C	1640	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	D	1640	-	3,3,3	0.50	0	2,2,2	0.31	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
2	EDO	B	1640	-	-	0/1/1/1	0/0/0/0
2	EDO	C	1640	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1640	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1640	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	458/467 (98%)	0.26	8 (1%) 70 76	26, 38, 65, 80	3 (0%)
1	B	458/467 (98%)	0.23	12 (2%) 56 64	26, 41, 68, 81	2 (0%)
1	C	458/467 (98%)	0.53	33 (7%) 16 21	25, 51, 93, 100	3 (0%)
1	D	457/467 (97%)	0.43	33 (7%) 16 21	25, 57, 84, 100	1 (0%)
All	All	1831/1868 (98%)	0.36	86 (4%) 32 40	25, 45, 79, 100	9 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	538	VAL	6.6
1	D	616	VAL	6.5
1	C	537	ASN	5.6
1	C	530[A]	TRP	5.4
1	D	536	VAL	5.1
1	C	539	GLY	5.0
1	D	620	LEU	4.8
1	D	382	LEU	4.5
1	C	588	TYR	4.5
1	C	275	LEU	4.4
1	C	542	LEU	4.4
1	D	530	TRP	4.3
1	C	613	CYS	4.3
1	A	271	ARG	4.2
1	C	614	ASP	4.2
1	C	543	THR	4.1
1	C	548	VAL	4.1
1	C	616	VAL	4.1
1	D	540	ALA	4.0
1	C	620	LEU	3.8
1	D	542	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	182	MET	3.7
1	C	639	ALA	3.6
1	B	538	VAL	3.6
1	C	617	GLU	3.5
1	A	382	LEU	3.4
1	C	538	VAL	3.4
1	C	540	ALA	3.3
1	C	565	LEU	3.3
1	C	615	SER	3.2
1	C	527	PRO	3.2
1	D	268	ILE	3.2
1	B	539	GLY	3.2
1	A	268	ILE	3.2
1	D	614	ASP	3.1
1	D	537	ASN	3.1
1	B	271	ARG	3.1
1	D	585	LEU	3.1
1	A	532	ALA	3.1
1	A	539	GLY	3.0
1	C	562	GLY	3.0
1	C	529	ARG	3.0
1	C	611	LEU	3.0
1	C	544	THR	3.0
1	B	268	ILE	2.9
1	C	541	GLN	2.9
1	D	563	GLY	2.8
1	C	564	HIS	2.8
1	A	269	ASN	2.8
1	B	530	TRP	2.7
1	B	537	ASN	2.7
1	C	528	ILE	2.7
1	D	377	PHE	2.7
1	C	618	ASP	2.6
1	C	536	VAL	2.6
1	D	465	GLN	2.6
1	A	540	ALA	2.6
1	D	543	THR	2.6
1	C	268	ILE	2.5
1	D	615	SER	2.5
1	B	411	ASP	2.5
1	D	545	GLU	2.5
1	D	564	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	617	GLU	2.4
1	B	529	ARG	2.3
1	D	608	VAL	2.3
1	C	622	LEU	2.3
1	B	307	THR	2.2
1	C	546	THR	2.2
1	D	565	LEU	2.2
1	D	266	ARG	2.2
1	D	639	ALA	2.2
1	D	275	LEU	2.2
1	D	186[A]	ARG	2.2
1	D	611	LEU	2.2
1	D	269	ASN	2.1
1	B	528	ILE	2.1
1	D	396	LEU	2.1
1	D	337	PHE	2.1
1	B	382	LEU	2.1
1	D	607	ARG	2.1
1	D	623	ALA	2.1
1	D	622	LEU	2.1
1	B	639	ALA	2.1
1	C	587	ILE	2.0
1	A	530	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	C	1640	4/4	0.94	0.20	6.70	42,47,48,50	0
2	EDO	B	1640	4/4	0.96	0.18	5.47	33,38,39,39	0
2	EDO	D	1640	4/4	0.94	0.12	0.48	49,52,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.