



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:26 AM UTC

PDB ID : 4CCK / pdb_00004cck
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 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

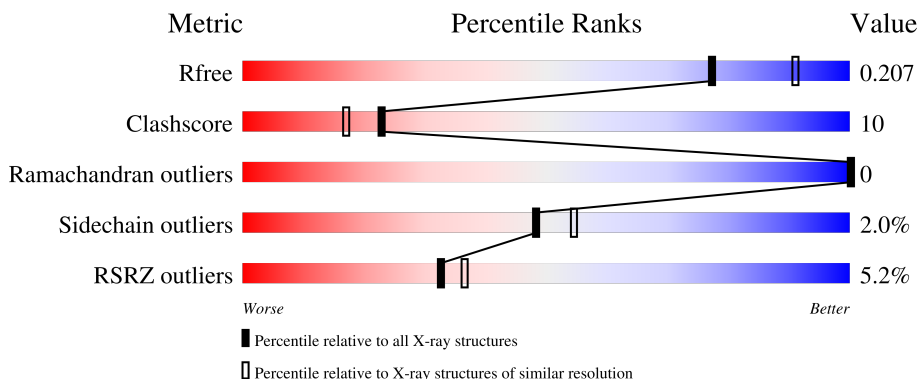
1 Overall quality at a glance

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of 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	2% 78% 18% ..
1	B	467	8% 74% 21% ..
1	C	467	4% 81% 15% ..
1	D	467	6% 70% 26% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15509 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	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 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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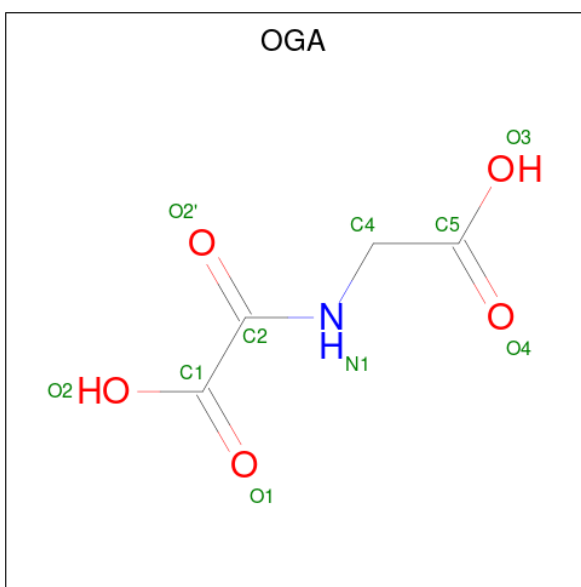
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Chain	Residue	Modelled	Actual	Comment	Reference
C	643	GLU	-	expression tag	UNP Q9H6W3
C	644	ASN	-	expression tag	UNP Q9H6W3
C	645	LEU	-	expression tag	UNP Q9H6W3
C	646	TYR	-	expression tag	UNP Q9H6W3
C	647	PHE	-	expression tag	UNP Q9H6W3
C	648	GLN	-	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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

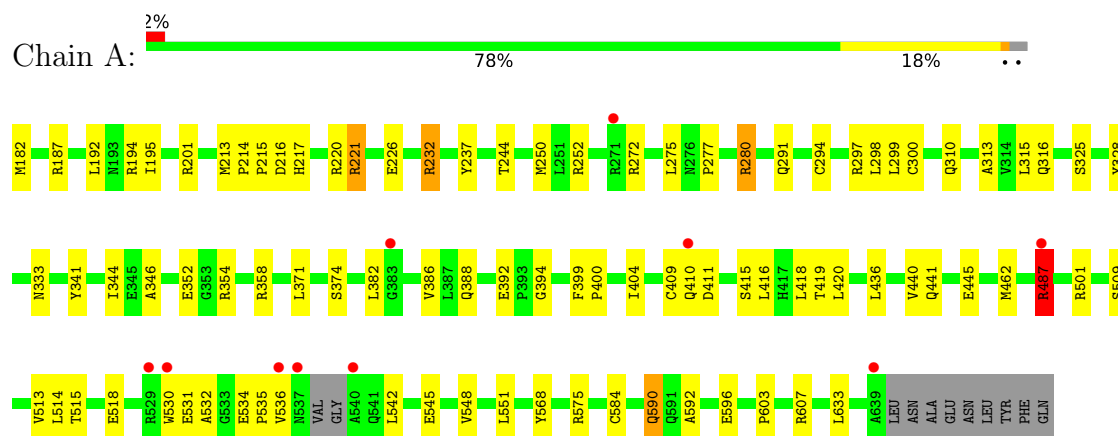
- Molecule 5 is water.

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

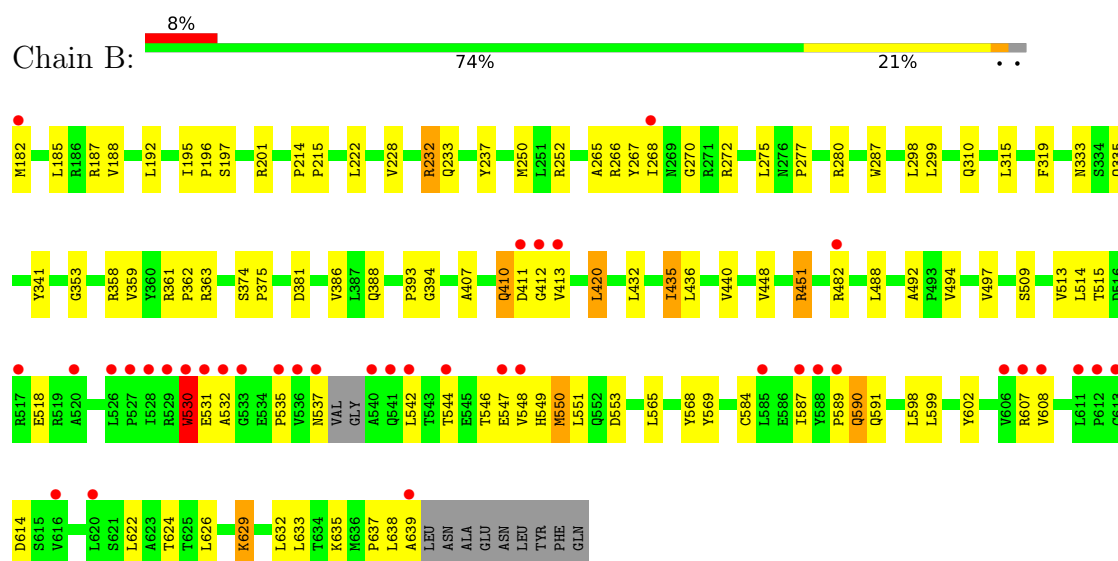
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

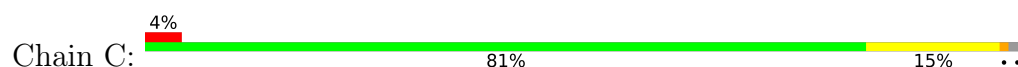
• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

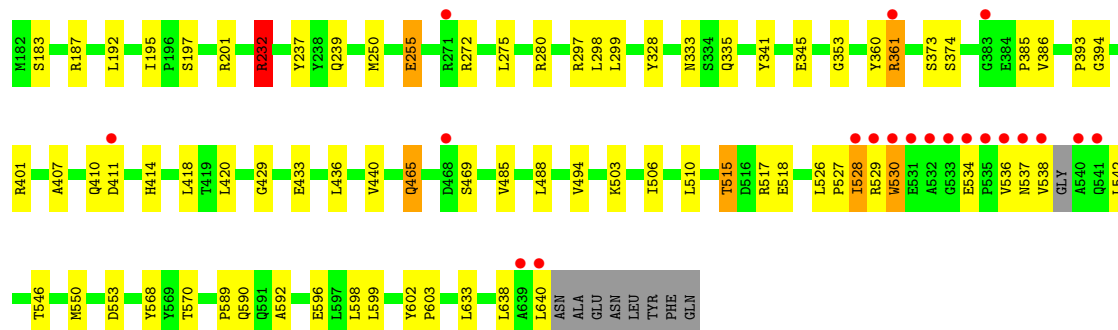


• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66

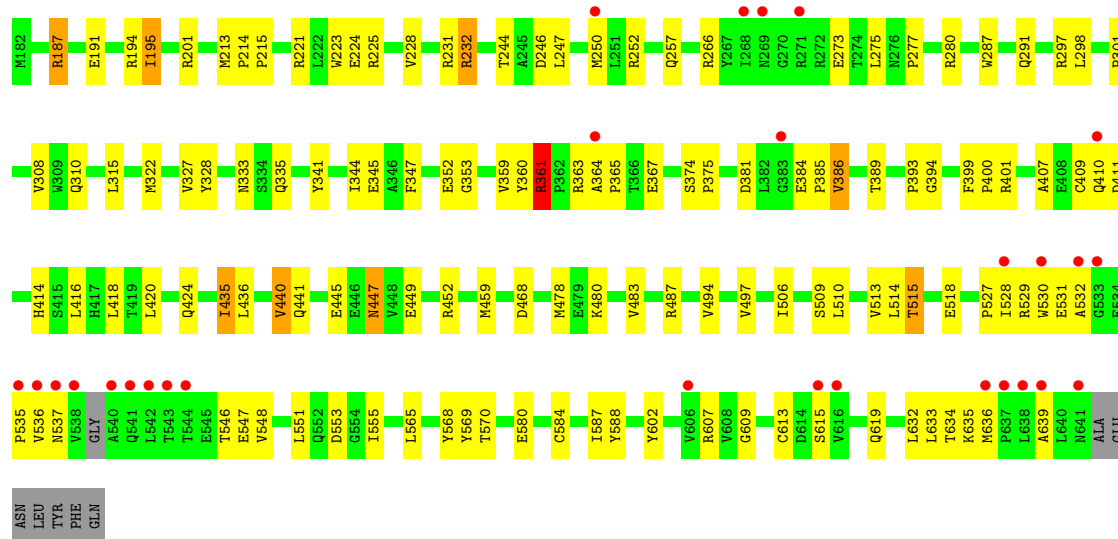


• Molecule 1: BIFUNCTIONAL LYSINE-SPECIFIC DEMETHYLASE AND HISTIDYL-HYDROXYLASE NO66





• 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	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 0.199 , 0.207	Depositor DCC
R_{free} test set	6595 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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, OGA, MN

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	0/3762	0.90	11/5117 (0.2%)
1	B	0.41	0/3749	0.88	5/5106 (0.1%)
1	C	0.41	0/3769	0.90	12/5131 (0.2%)
1	D	0.37	0/3757	0.87	12/5116 (0.2%)
All	All	0.40	0/15037	0.89	40/20470 (0.2%)

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 (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	GLY	N-CA-C	9.41	127.45	115.21
1	D	361[A]	ARG	CA-C-O	-7.99	111.62	120.25
1	D	361[B]	ARG	CA-C-O	-7.99	111.62	120.25
1	D	187[A]	ARG	N-CA-C	7.33	120.14	111.71
1	D	187[B]	ARG	N-CA-C	7.33	120.14	111.71
1	C	299	LEU	N-CA-C	7.21	120.19	111.82
1	A	299	LEU	N-CA-C	6.84	119.75	111.82
1	B	614	ASP	N-CA-C	6.73	118.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	ILE	CA-C-N	6.24	125.98	119.05
1	D	195	ILE	C-N-CA	6.24	125.98	119.05
1	C	386	VAL	N-CA-C	-6.11	105.70	113.22
1	A	487[A]	ARG	CA-C-O	-6.11	114.08	120.55
1	A	487[B]	ARG	CA-C-O	-6.11	114.08	120.55
1	C	515	THR	N-CA-C	-6.05	102.72	110.53
1	C	361[A]	ARG	CA-C-O	-6.02	113.75	120.25
1	C	361[B]	ARG	CA-C-O	-6.02	113.75	120.25
1	A	509	SER	N-CA-C	5.98	118.48	110.35
1	C	530	TRP	N-CA-C	5.86	118.21	109.25
1	B	299	LEU	N-CA-C	5.77	119.58	112.54
1	A	548	VAL	CB-CA-C	-5.64	100.32	110.48
1	D	515	THR	N-CA-C	-5.62	103.28	110.53
1	C	469	SER	CB-CA-C	-5.59	101.94	109.71
1	C	232	ARG	N-CA-C	5.48	117.34	111.36
1	A	575	ARG	N-CA-C	-5.34	106.71	113.18
1	A	487[A]	ARG	N-CA-C	-5.27	105.53	111.28
1	A	487[B]	ARG	N-CA-C	-5.27	105.53	111.28
1	A	226	GLU	N-CA-C	5.24	117.03	109.07
1	C	469	SER	N-CA-C	5.19	118.00	110.42
1	A	221	ARG	N-CA-C	5.18	120.60	113.97
1	D	510	LEU	N-CA-C	-5.18	102.68	110.24
1	D	509	SER	N-CA-C	5.16	117.78	110.50
1	C	494	VAL	N-CA-C	5.12	115.84	110.62
1	D	386	VAL	N-CA-C	-5.11	106.07	113.07
1	D	588	TYR	CA-C-N	5.06	126.17	119.84
1	D	588	TYR	C-N-CA	5.06	126.17	119.84
1	A	346	ALA	N-CA-C	5.04	117.71	109.59
1	C	510	LEU	N-CA-C	-5.04	102.88	110.24
1	B	509	SER	N-CA-C	5.02	117.58	110.50
1	C	528	ILE	CB-CA-C	-5.01	103.07	111.29
1	B	319	PHE	N-CA-C	-5.01	106.33	112.90

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

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Mol	Chain	Res	Type	Group
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 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	3662	0	3583	71	0
1	B	3641	0	3554	94	0
1	C	3663	0	3571	64	0
1	D	3654	0	3553	100	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	302	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 (302) 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:448:VAL:HG23	1:B:451:ARG:HH12	1.34	0.93
1:A:182:MET:HE3	1:A:187:ARG:HH11	1.42	0.83
1:D:247:LEU:HA	1:D:250:MET:HE2	1.63	0.81
1:A:232:ARG:HD2	1:A:394:GLY:O	1.82	0.80
1:C:550:MET:HE3	1:C:599:LEU:HD23	1.63	0.79
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:B:410:GLN:HA	1:B:410:GLN:HE21	1.56	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:A:232:ARG:HD3	1:A:237:TYR:CD2	2.27	0.69
1:D:250:MET:HE1	1:D:298:LEU:HD22	1.74	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:HE21	1:D:410:GLN:HA	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:550:MET:HE3	1:B:599:LEU:HD23	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:A:250:MET:HE1	1:A:298:LEU:HD21	1.81	0.63
1:C:436:LEU:CD1	1:D:440[B]:VAL:CG2	2.77	0.63
1:B:250:MET:HE1	1:B:298:LEU:HD11	1.81	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:436:LEU:HD12	1:D:440[B]:VAL:CG2	2.33	0.59
1:C:542:LEU:HD23	1:C:638:LEU:HD21	1.84	0.59
1:B:590:GLN:H	1:B:590:GLN:CD	2.09	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:B:267:TYR:C	1:B:268:ILE:HD12	2.30	0.57
1:C:436:LEU:HD11	1:D:440[B]:VAL:HG22	1.87	0.57
1:B:333:ASN:CG	1:B:411:ASP:HA	2.30	0.56
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:HH11	1:A:220:ARG:HG3	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:HH11	1:B:451:ARG:HB2	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:C:250:MET:HE1	1:C:298:LEU:HD21	1.88	0.55
1:B:268:ILE:HD11	5:B:2051:HOH:O	2.06	0.55
1:B:451:ARG:HH11	1:B:451:ARG:CB	2.20	0.55
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:C:420:LEU:C	1:C:420:LEU:HD23	2.33	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:HB3	1.89	0.53
1:B:633:LEU:HD12	1:B:633:LEU:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:MET:HE1	1:C:598:LEU:HB3	1.91	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:A:418:LEU:C	1:A:418:LEU:HD23	2.34	0.53
1:D:506:ILE:HG23	1:D:570:THR:CG2	2.39	0.53
1:A:633:LEU:C	1:A:633:LEU:HD12	2.33	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
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:333:ASN:OD1	1:B:411:ASP:HA	2.10	0.52
1:C:275:LEU:N	1:C:275:LEU:HD12	2.25	0.52
1:D:213:MET:HE1	1:D:228:VAL:HG11	1.91	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:B:530[B]:TRP:HZ2	1:D:414:HIS:NE2	2.08	0.51
1:C:515:THR:OG1	1:C:518:GLU:HG3	2.10	0.51
1:C:590:GLN:CD	1:C:590:GLN:H	2.18	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:250:MET:HE1	1:D:298:LEU:CD2	2.39	0.51
1:D:363:ARG:NH1	1:D:381:ASP:HB3	2.26	0.51
1:A:182:MET:HE3	1:A:187:ARG:NH1	2.18	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:HG2	1:C:361[A]:ARG:HH11	1.75	0.50
1:D:301:PRO:HG2	1:D:327:VAL:HG23	1.93	0.50
1:A:410:GLN:HA	1:A:410:GLN:NE2	2.24	0.50
1:B:232:ARG:HD3	1:B:237:TYR:CD2	2.46	0.50
1:D:275:LEU:HD12	1:D:275:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:550:MET:HE3	1:B:599:LEU:CD2	2.41	0.49
1:A:590:GLN:CD	1:A:590:GLN:H	2.20	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: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: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:D:633:LEU:HD12	1:D:633:LEU:C	2.38	0.48
1:D:555:ILE:O	1:D:569:TYR:HA	2.14	0.48
1:A:462:MET:HE2	1:B:494:VAL:HG12	1.95	0.48
1:B:187:ARG:HG2	1:B:187:ARG:HH11	1.79	0.48
1:B:275:LEU:HD12	1:B:275:LEU:N	2.29	0.48
1:D:436:LEU:O	1:D:440[A]:VAL:HG22	2.14	0.48
1:A:275:LEU:N	1:A:275:LEU:HD12	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:D:418:LEU:C	1:D:418:LEU:HD23	2.39	0.48
1:C:297:ARG:HD3	1:C:328:TYR:CE2	2.49	0.48
1:D:247:LEU:HA	1:D:250:MET:CE	2.40	0.48
1:D:266:ARG:O	1:D:273:GLU:HG2	2.14	0.47
1:C:633:LEU:C	1:C:633:LEU:HD12	2.38	0.47
1:D:333:ASN:CG	1:D:411:ASP:HA	2.39	0.47
1:D:345:GLU:OE2	1:D:401:ARG:HG2	2.13	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:C:333:ASN:CG	1:C:411:ASP:HA	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:B:633:LEU:O	2.15	0.47
1:D:536:VAL:HG12	1:D:536:VAL:O	2.15	0.47
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:A:462:MET:HE2	1:B:494:VAL:CG1	2.46	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
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:B:549:HIS:C	1:B:632:LEU:HD12	2.42	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:B:565:LEU:HB2	1:B:587:ILE:O	2.17	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:HA	1:B:410:GLN:NE2	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:H	1:C:640:LEU:HD23	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:537:ASN:CB	1:D:291:GLN:HE22	2.31	0.44
1:B:546:THR:O	1:B:607:ARG:HA	2.18	0.44
1:D:528:ILE:N	1:D:528:ILE:HD12	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:182:MET:CE	1:A:187:ARG:HH11	2.23	0.44
1:A:515:THR:OG1	1:A:518:GLU:HG3	2.17	0.44
1:D:635:LYS:O	1:D:636:MET:HE3	2.18	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:A:436:LEU:O	1:A:440:VAL:HG23	2.17	0.43
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:333:ASN:CG	1:A:411:ASP:HA	2.43	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:B:195:ILE:HA	1:B:196:PRO:HD3	1.89	0.43
1:B:451:ARG:NH1	1:B:451:ARG:HB2	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: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: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:436:LEU:HD12	1:B:440[B]:VAL:CG2	2.49	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:C:418:LEU:C	1:C:418:LEU:HD23	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:VAL:O	1:C:488:LEU:HB2	2.19	0.42
1:C:550:MET:HE1	1:C:598:LEU:CB	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:A:542:LEU:HD12	1:A:542:LEU:N	2.35	0.42
1:B:250:MET:HE2	1:B:250:MET:HB3	1.92	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:315:LEU:CD1	1:B:420:LEU:HD11	2.49	0.42
1:B:359:VAL:O	1:B:386:VAL:HG12	2.20	0.42
1:B:637:PRO:C	1:B:639:ALA:H	2.26	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
1:B:550:MET:HE1	1:B:598:LEU:CB	2.50	0.42
1:D:449:GLU:CD	1:D:452:ARG:HE	2.27	0.42
1:B:361:ARG:O	1:B:362:PRO:C	2.62	0.41
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:A:291:GLN:HE22	1:C:538:VAL:CB	2.34	0.41
1:B:549:HIS:CE1	1:B:633:LEU:HD11	2.56	0.41
1:B:553:ASP:HB2	1:B:602:TYR:CE1	2.56	0.41
1:C:373:SER:HB3	5:C:2096:HOH:O	2.21	0.41
1:C:550:MET:CE	1:C:598:LEU:HB3	2.50	0.41
1:D:221:ARG:O	1:D:225:ARG:HD2	2.20	0.41
1:D:548:VAL:HG21	1:D:632:LEU:HD21	2.03	0.41
1:C:272:ARG:HH11	1:C:272:ARG:HG3	1.85	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:382:LEU:HD22	1:A:404:ILE:HG21	2.04	0.40
1:A:399:PHE:HA	1:A:400:PRO:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:589:PRO:C	1:B:591:GLN:H	2.30	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 [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%)	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 [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	388/399 (97%)	383 (99%)	5 (1%)	61	68
1	B	382/399 (96%)	369 (97%)	13 (3%)	32	33
1	C	386/399 (97%)	379 (98%)	7 (2%)	51	58
1	D	383/399 (96%)	374 (98%)	9 (2%)	44	49
All	All	1539/1596 (96%)	1505 (98%)	34 (2%)	48	51

All (34) 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	590	GLN
1	A	603	PRO
1	B	182	MET
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	629	LYS
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	194	ARG
1	D	232	ARG
1	D	409	CYS

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Mol	Chain	Res	Type
1	D	435	ILE
1	D	440[A]	VAL
1	D	440[B]	VAL
1	D	447	ASN
1	D	478	MET
1	D	580	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	257	GLN
1	A	260	GLN
1	A	291	GLN
1	A	310	GLN
1	A	333	ASN
1	A	376	ASN
1	A	388	GLN
1	A	410	GLN
1	A	465	GLN
1	A	500	GLN
1	A	537	ASN
1	B	239	GLN
1	B	257	GLN
1	B	326	ASN
1	B	376	ASN
1	B	388	GLN
1	B	410	GLN
1	B	424	GLN
1	B	552	GLN
1	B	564	HIS
1	B	590	GLN
1	C	253	ASN
1	C	260	GLN
1	C	269	ASN
1	C	310	GLN
1	C	335	GLN
1	C	379	GLN
1	C	406	GLN
1	C	414	HIS
1	C	424	GLN
1	C	590	GLN

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Mol	Chain	Res	Type
1	D	217	HIS
1	D	253	ASN
1	D	257	GLN
1	D	260	GLN
1	D	291	GLN
1	D	379	GLN
1	D	406	GLN
1	D	410	GLN
1	D	417	HIS
1	D	424	GLN
1	D	447	ASN
1	D	466	HIS
1	D	500	GLN
1	D	564	HIS
1	D	590	GLN
1	D	591	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	EDO	C	903	-	3,3,3	0.38	0	2,2,2	0.39	0
4	EDO	D	903	-	3,3,3	0.40	0	2,2,2	0.38	0
3	OGA	A	902	2	9,9,9	1.09	0	8,11,11	1.14	1 (12%)
3	OGA	C	902	2	9,9,9	1.10	0	8,11,11	1.14	1 (12%)
4	EDO	B	903	-	3,3,3	0.39	0	2,2,2	0.38	0
3	OGA	B	902	2	9,9,9	1.11	0	8,11,11	1.15	1 (12%)
4	EDO	A	903	-	3,3,3	0.45	0	2,2,2	0.32	0
3	OGA	D	902	2	9,9,9	1.09	0	8,11,11	1.14	1 (12%)

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	EDO	C	903	-	-	0/1/1/1	-
4	EDO	D	903	-	-	1/1/1/1	-
3	OGA	A	902	2	-	0/8/9/9	-
3	OGA	C	902	2	-	0/8/9/9	-
4	EDO	B	903	-	-	0/1/1/1	-
3	OGA	B	902	2	-	0/8/9/9	-
4	EDO	A	903	-	-	0/1/1/1	-
3	OGA	D	902	2	-	0/8/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	OGA	O2'-C2-C1	-2.18	118.49	121.36
3	D	902	OGA	O2'-C2-C1	-2.17	118.51	121.36
3	C	902	OGA	O2'-C2-C1	-2.16	118.52	121.36
3	A	902	OGA	O2'-C2-C1	-2.15	118.52	121.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	903	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	456/467 (97%)	-0.04	10 (2%) 62 66	22, 34, 58, 78	3 (0%)
1	B	456/467 (97%)	0.46	38 (8%) 17 19	17, 41, 85, 100	7 (1%)
1	C	458/467 (98%)	0.09	20 (4%) 39 44	23, 36, 62, 93	6 (1%)
1	D	459/467 (98%)	0.44	28 (6%) 27 31	21, 45, 80, 100	3 (0%)
All	All	1829/1868 (97%)	0.24	96 (5%) 33 36	17, 39, 73, 100	19 (1%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	536	VAL	7.3
1	B	530[A]	TRP	7.1
1	C	532	ALA	6.6
1	C	530	TRP	6.4
1	C	640	LEU	6.2
1	B	537	ASN	6.1
1	C	528	ILE	5.8
1	B	532	ALA	5.3
1	D	538	VAL	5.2
1	C	538	VAL	5.0
1	D	641	ASN	4.9
1	B	531	GLU	4.7
1	A	540	ALA	4.6
1	B	540	ALA	4.5
1	C	535	PRO	4.5
1	D	536	VAL	4.4
1	A	639	ALA	4.3
1	C	536	VAL	4.2
1	C	529	ARG	4.1
1	B	612	PRO	4.1
1	D	537	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	535	PRO	4.0
1	C	531	GLU	3.9
1	D	540	ALA	3.8
1	C	537	ASN	3.8
1	C	411	ASP	3.5
1	B	616	VAL	3.5
1	B	411	ASP	3.5
1	A	536	VAL	3.5
1	C	540	ALA	3.4
1	D	530	TRP	3.4
1	A	537	ASN	3.3
1	C	271	ARG	3.3
1	C	533	GLY	3.2
1	B	533	GLY	3.1
1	B	588	TYR	3.1
1	B	613	CYS	3.1
1	D	410	GLN	3.0
1	B	608	VAL	3.0
1	B	412	GLY	3.0
1	D	542	LEU	2.9
1	B	517	ARG	2.9
1	D	615	SER	2.8
1	B	589	PRO	2.8
1	D	528	ILE	2.8
1	C	639	ALA	2.8
1	B	527	PRO	2.8
1	B	528	ILE	2.8
1	B	587	ILE	2.8
1	D	268	ILE	2.8
1	D	636	MET	2.8
1	D	639	ALA	2.8
1	D	541	GLN	2.7
1	B	542	LEU	2.7
1	D	638	LEU	2.7
1	B	639	ALA	2.7
1	B	620	LEU	2.7
1	A	410	GLN	2.6
1	D	533	GLY	2.6
1	D	616	VAL	2.5
1	A	271	ARG	2.5
1	D	271	ARG	2.5
1	C	534	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	487[A]	ARG	2.5
1	B	529	ARG	2.5
1	D	383	GLY	2.5
1	B	606	VAL	2.4
1	B	413	VAL	2.4
1	B	526	LEU	2.4
1	D	544	THR	2.3
1	B	585	LEU	2.3
1	C	383	GLY	2.3
1	D	269	ASN	2.3
1	D	364	ALA	2.3
1	B	607	ARG	2.3
1	A	529	ARG	2.3
1	B	611	LEU	2.3
1	D	535	PRO	2.2
1	D	532	ALA	2.2
1	B	548	VAL	2.2
1	C	361[A]	ARG	2.2
1	A	383	GLY	2.2
1	C	468[A]	ASP	2.2
1	B	268	ILE	2.1
1	D	606	VAL	2.1
1	B	541	GLN	2.1
1	D	543	THR	2.1
1	D	637	PRO	2.1
1	B	482[A]	ARG	2.1
1	B	520	ALA	2.1
1	B	547	GLU	2.1
1	B	544	THR	2.1
1	C	541	GLN	2.0
1	B	182	MET	2.0
1	D	250	MET	2.0
1	A	530	TRP	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	OGA	D	902	10/10	0.92	0.10	52,54,57,57	0
3	OGA	B	902	10/10	0.93	0.09	37,43,47,48	0
3	OGA	C	902	10/10	0.94	0.09	38,40,46,47	0
3	OGA	A	902	10/10	0.94	0.08	36,41,43,45	0
4	EDO	C	903	4/4	0.95	0.08	34,35,35,37	0
4	EDO	D	903	4/4	0.96	0.10	50,51,52,52	0
4	EDO	A	903	4/4	0.97	0.07	31,35,36,37	0
4	EDO	B	903	4/4	0.98	0.09	32,37,38,42	0
2	MN	A	901	1/1	1.00	0.07	18,18,18,18	0
2	MN	B	901	1/1	1.00	0.06	18,18,18,18	0
2	MN	C	901	1/1	1.00	0.08	20,20,20,20	0
2	MN	D	901	1/1	1.00	0.07	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.