



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:43 AM UTC

PDB ID : 4EZH / pdb_00004ezh
Title : the crystal structure of KDM6B bound with H3K27me3 peptide
Authors : Cheng, Z.J.; Patel, D.J.
Deposited on : 2012-05-02
Resolution : 2.52 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

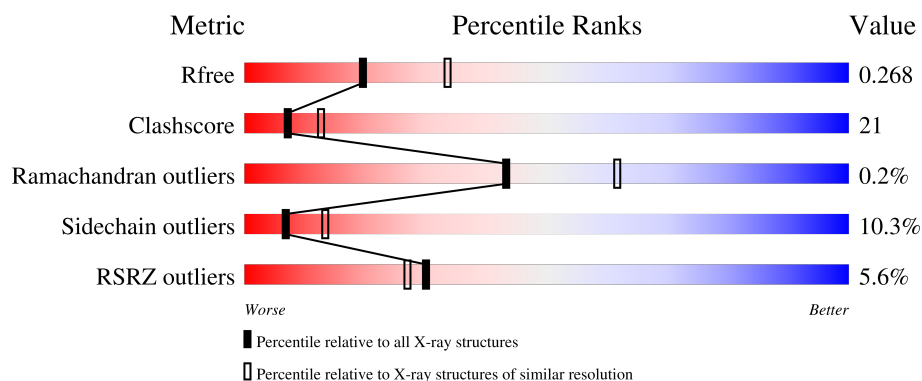
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	486	4% 57% 31% 5% 6%
1	B	486	5% 56% 31% 5% 7%
2	C	11	36% 55% 9% 36%
2	D	11	55% 64% 27% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7543 atoms, of which 8 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 Lysine-specific demethylase 6B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	0	0	0
			3668	2331	8	635	675	19			
1	B	451	Total	C	N	O	S		0	0	0
			3627	2313	629	666	19				

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1296	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1297	GLU	-	SEE REMARK 999	UNP Q5NCY0
A	1298	VAL	-	SEE REMARK 999	UNP Q5NCY0
A	1299	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1300	PHE	-	SEE REMARK 999	UNP Q5NCY0
A	1301	GLN	-	SEE REMARK 999	UNP Q5NCY0
A	1303	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1304	PRO	-	SEE REMARK 999	UNP Q5NCY0
A	1305	THR	-	SEE REMARK 999	UNP Q5NCY0
A	1306	LYS	-	SEE REMARK 999	UNP Q5NCY0
A	1307	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1308	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1309	ARG	-	SEE REMARK 999	UNP Q5NCY0
A	1310	LYS	-	SEE REMARK 999	UNP Q5NCY0
A	1311	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1312	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1313	PRO	-	SEE REMARK 999	UNP Q5NCY0
A	1314	ALA	-	SEE REMARK 999	UNP Q5NCY0
A	1315	THR	-	SEE REMARK 999	UNP Q5NCY0
A	1316	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1317	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1318	GLY	-	SEE REMARK 999	UNP Q5NCY0
A	1319	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1320	SER	-	SEE REMARK 999	UNP Q5NCY0
A	1321	GLY	-	SEE REMARK 999	UNP Q5NCY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1322	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1296	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1297	GLU	-	SEE REMARK 999	UNP Q5NCY0
B	1298	VAL	-	SEE REMARK 999	UNP Q5NCY0
B	1299	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1300	PHE	-	SEE REMARK 999	UNP Q5NCY0
B	1302	GLN	-	SEE REMARK 999	UNP Q5NCY0
B	1303	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1304	PRO	-	SEE REMARK 999	UNP Q5NCY0
B	1305	THR	-	SEE REMARK 999	UNP Q5NCY0
B	1306	LYS	-	SEE REMARK 999	UNP Q5NCY0
B	1307	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1308	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1309	ARG	-	SEE REMARK 999	UNP Q5NCY0
B	1310	LYS	-	SEE REMARK 999	UNP Q5NCY0
B	1311	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1312	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1313	PRO	-	SEE REMARK 999	UNP Q5NCY0
B	1314	ALA	-	SEE REMARK 999	UNP Q5NCY0
B	1315	THR	-	SEE REMARK 999	UNP Q5NCY0
B	1316	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1317	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1318	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1319	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1320	SER	-	SEE REMARK 999	UNP Q5NCY0
B	1321	GLY	-	SEE REMARK 999	UNP Q5NCY0
B	1322	SER	-	SEE REMARK 999	UNP Q5NCY0

- Molecule 2 is a protein called SYNTHESIZED methylation peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			71	43	15	13			
2	D	11	Total	C	N	O	0	0	0
			71	43	15	13			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

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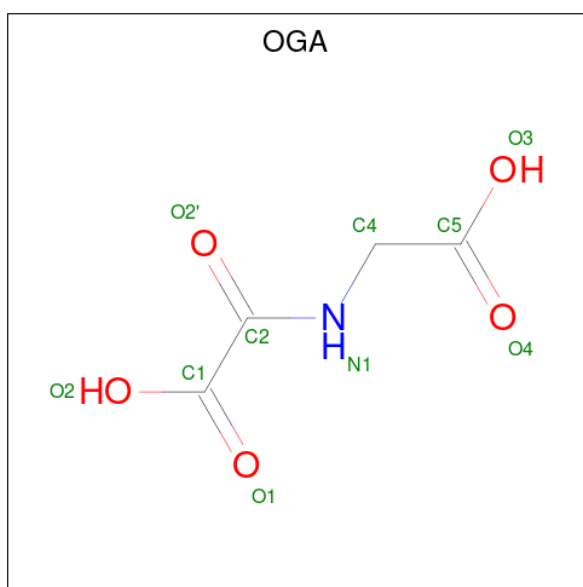
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ni 1 1	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



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

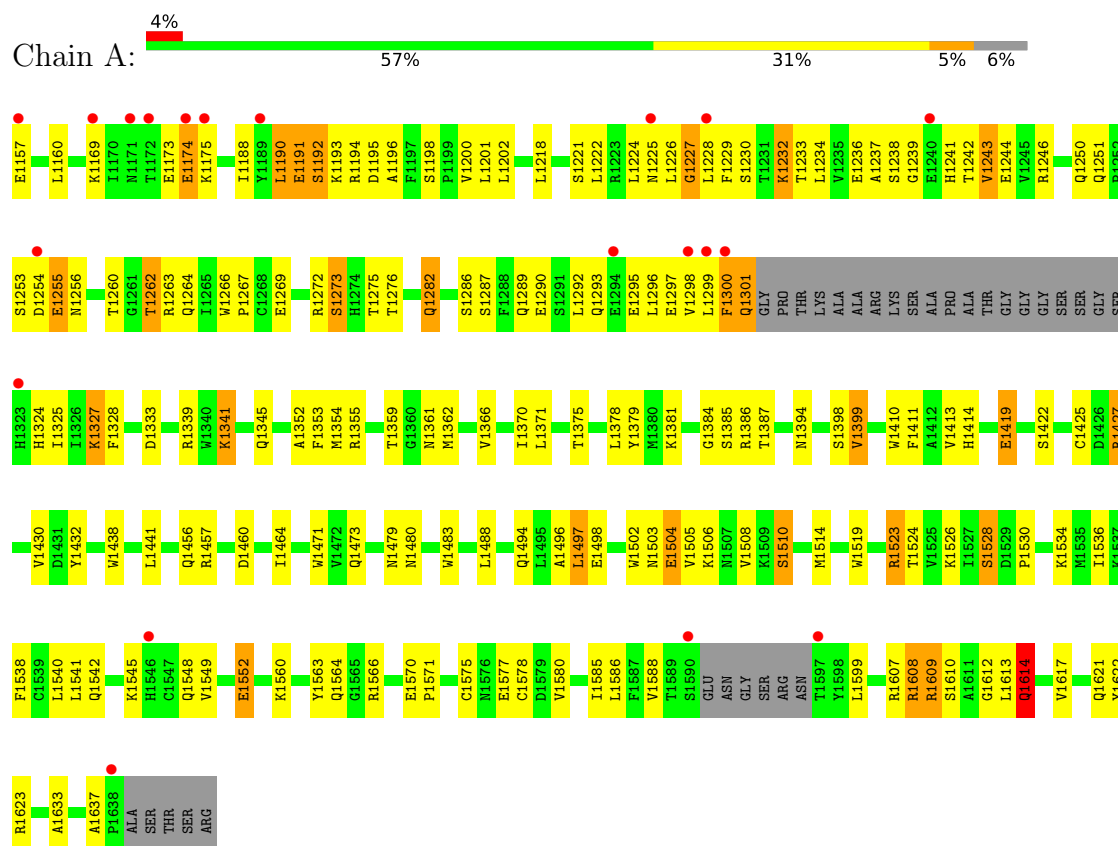
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	39	Total O 39 39	0	0

3 Residue-property plots

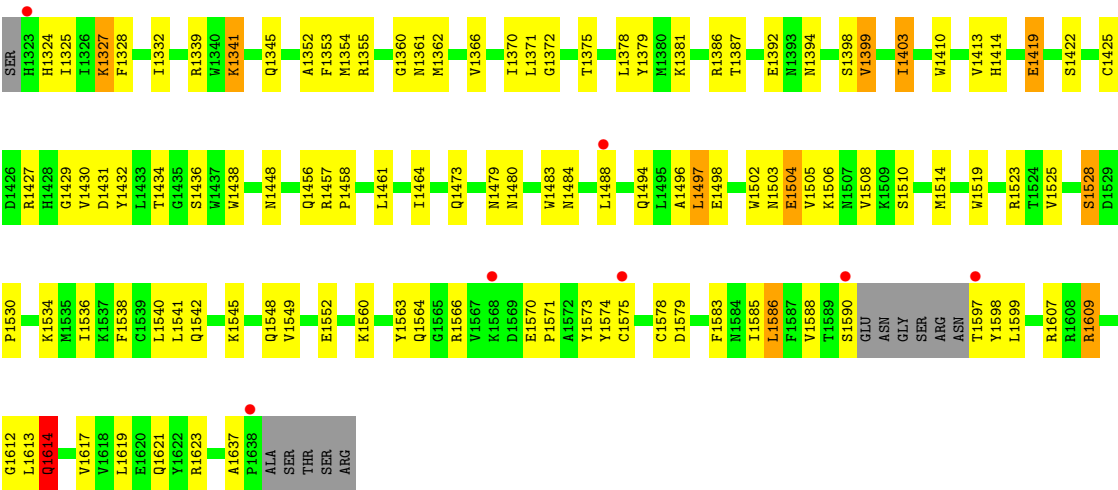
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lysine-specific demethylase 6B

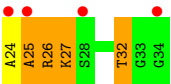


• Molecule 1: Lysine-specific demethylase 6B





● Molecule 2: SYNTHESIZED methylation peptide



● Molecule 2: SYNTHESIZED methylation peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.68Å 102.41Å 143.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.52 40.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-2.52) 87.6 (40.00-2.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.213 , 0.254 0.229 , 0.268	Depositor DCC
R_{free} test set	2113 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7543	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5396e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OGA, ZN, M3L, NI

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	0.72	0/3755	0.95	7/5110 (0.1%)
1	B	0.74	1/3721 (0.0%)	0.95	9/5062 (0.2%)
2	C	1.76	1/59 (1.7%)	1.55	1/79 (1.3%)
2	D	0.51	0/59	0.94	0/79
All	All	0.74	2/7594 (0.0%)	0.95	17/10330 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	25	ALA	CA-CB	-6.29	1.43	1.53
1	B	1473	GLN	C-O	-6.10	1.16	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1254	ASP	N-CA-C	8.77	120.92	111.36
1	B	1255	GLU	N-CA-C	8.70	122.76	110.50
2	C	25	ALA	N-CA-C	-7.32	99.20	110.10
1	A	1514	MET	N-CA-C	6.16	118.78	111.33
1	A	1237	ALA	N-CA-C	-5.88	104.22	111.40
1	A	1190	LEU	N-CA-C	5.87	118.29	107.73
1	A	1327	LYS	CB-CG-CD	5.75	124.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1275	THR	CB-CA-C	-5.75	101.97	114.10
1	A	1608	ARG	N-CA-C	-5.57	106.18	112.87
1	A	1614	GLN	CA-CB-CG	5.55	125.21	114.10
1	B	1193	LYS	N-CA-C	-5.37	106.57	113.23
1	B	1514	MET	N-CA-C	5.34	117.80	111.33
1	B	1327	LYS	CB-CG-CD	5.30	123.50	111.30
1	B	1614	GLN	CA-CB-CG	5.19	124.47	114.10
1	A	1255	GLU	N-CA-C	5.18	117.26	109.23
1	B	1574	TYR	N-CA-C	-5.12	101.29	109.23
1	B	1573	TYR	N-CA-C	5.11	117.57	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1174	GLU	Peptide

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	3660	8	3580	153	1
1	B	3627	0	3551	153	0
2	C	71	0	76	6	0
2	D	71	0	76	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	3	0	0
5	B	10	0	3	0	0
6	A	43	0	0	4	0
6	B	39	0	0	2	0
All	All	7535	8	7289	307	1

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 21.

All (307) 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:1251:GLN:NE2	1:B:1256:ASN:HA	1.32	1.43
1:B:1403:ILE:HG23	1:B:1479:ASN:O	1.48	1.13
1:B:1157:GLU:OE1	1:B:1157:GLU:HA	1.48	1.09
1:A:1160:LEU:HD11	1:A:1497:LEU:HB3	1.35	1.08
1:B:1597:THR:HG22	1:B:1598:TYR:H	1.16	1.07
1:B:1160:LEU:HD11	1:B:1497:LEU:HB3	1.34	1.06
1:A:1251:GLN:HE22	1:A:1256:ASN:HA	1.18	1.06
1:B:1219:ALA:HA	1:B:1224:LEU:HD13	1.37	1.06
1:A:1300:PHE:O	1:A:1301:GLN:NE2	1.91	1.04
1:B:1251:GLN:NE2	1:B:1256:ASN:CA	2.21	1.02
1:B:1247:THR:HB	1:B:1271:SER:HB3	1.37	1.01
1:A:1174:GLU:OE2	1:A:1174:GLU:HA	1.54	0.99
1:B:1614:GLN:OE1	1:B:1614:GLN:N	1.96	0.97
1:B:1251:GLN:HE22	1:B:1256:ASN:CA	1.76	0.96
1:A:1614:GLN:N	1:A:1614:GLN:OE1	1.99	0.94
1:B:1251:GLN:HE22	1:B:1256:ASN:HA	1.12	0.93
1:A:1193:LYS:HG2	1:A:1221:SER:O	1.69	0.92
1:B:1597:THR:HG22	1:B:1598:TYR:N	1.86	0.90
1:B:1403:ILE:CG2	1:B:1479:ASN:O	2.23	0.86
1:B:1300:PHE:CD1	1:B:1300:PHE:N	2.39	0.85
1:B:1193:LYS:HG3	1:B:1221:SER:O	1.77	0.84
1:A:1222:LEU:HB2	1:A:1224:LEU:HD11	1.60	0.84
1:A:1251:GLN:NE2	1:A:1256:ASN:HA	1.93	0.84
1:B:1398:SER:HB3	1:B:1464:ILE:HD13	1.61	0.83
1:B:1188:ILE:HD11	1:B:1204:PHE:CE2	2.13	0.82
1:A:1253:SER:HA	1:A:1473:GLN:OE1	1.79	0.82
1:B:1251:GLN:HE21	1:B:1256:ASN:HA	1.44	0.82
1:B:1300:PHE:N	1:B:1300:PHE:HD1	1.75	0.82
1:A:1398:SER:HB3	1:A:1464:ILE:HD13	1.61	0.81
1:A:1371:LEU:HB2	2:C:26:ARG:HB2	1.63	0.80
1:B:1157:GLU:OE1	1:B:1157:GLU:CA	2.29	0.79
1:A:1222:LEU:HB2	1:A:1224:LEU:CD1	2.12	0.79
1:B:1176:LEU:HD12	1:B:1177:PRO:HD2	1.66	0.78
1:A:1300:PHE:N	1:A:1300:PHE:HD1	1.81	0.77
1:A:1352:ALA:HA	1:A:1355:ARG:HE	1.46	0.77
1:A:1228:LEU:O	1:A:1233:THR:HB	1.85	0.77
1:B:1352:ALA:HA	1:B:1355:ARG:HE	1.49	0.77
1:A:1300:PHE:N	1:A:1300:PHE:CD1	2.53	0.75
1:A:1523:ARG:HG2	1:A:1524:THR:HG23	1.70	0.73
1:B:1403:ILE:HG23	1:B:1479:ASN:C	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:GLU:HG2	1:A:1192:SER:N	2.05	0.71
1:B:1222:LEU:HB2	1:B:1224:LEU:HD11	1.71	0.71
1:B:1193:LYS:CD	1:B:1193:LYS:N	2.53	0.71
1:A:1333:ASP:OD2	2:C:26:ARG:NH1	2.23	0.70
1:B:1193:LYS:N	1:B:1193:LYS:HD2	2.06	0.70
1:A:1272:ARG:HG2	1:A:1273:SER:N	2.06	0.69
1:A:1386:ARG:HG2	1:A:1438:TRP:CZ3	2.27	0.69
2:D:26:ARG:NH1	2:D:26:ARG:HG2	2.06	0.69
1:A:1289:GLN:HG3	1:A:1290:GLU:N	2.07	0.68
1:A:1227:GLY:O	1:A:1230:SER:HB3	1.94	0.68
1:B:1224:LEU:HD12	1:B:1224:LEU:N	2.07	0.68
1:B:1541:LEU:HG	1:B:1545:LYS:HE3	1.76	0.68
1:A:1296:LEU:HD23	1:A:1299:LEU:HD12	1.75	0.68
1:A:1238:SER:OG	1:A:1241:HIS:HB2	1.94	0.68
1:A:1295:GLU:O	1:A:1299:LEU:HG	1.94	0.67
1:B:1590:SER:HA	1:B:1597:THR:O	1.94	0.67
1:A:1193:LYS:CG	1:A:1221:SER:O	2.42	0.67
2:D:26:ARG:HG2	2:D:26:ARG:HH11	1.59	0.67
1:A:1296:LEU:HA	1:A:1299:LEU:HD12	1.77	0.67
1:A:1541:LEU:HG	1:A:1545:LYS:HE3	1.77	0.66
1:B:1575:CYS:HB3	1:B:1579:ASP:H	1.60	0.66
1:A:1353:PHE:CZ	1:A:1354:MET:HE3	2.31	0.66
1:B:1597:THR:CG2	1:B:1598:TYR:H	1.93	0.65
2:D:26:ARG:NH1	2:D:27:M3L:O	2.30	0.65
1:B:1386:ARG:HG2	1:B:1438:TRP:CZ3	2.31	0.65
1:A:1244:GLU:OE2	1:A:1246:ARG:NH1	2.30	0.64
1:A:1566:ARG:NH2	1:A:1570:GLU:O	2.30	0.64
6:B:1839:HOH:O	2:D:24:ALA:N	2.29	0.64
1:A:1612:GLY:C	1:A:1614:GLN:OE1	2.40	0.64
2:D:26:ARG:HH11	2:D:26:ARG:CG	2.11	0.64
1:B:1176:LEU:HB3	1:B:1448:ASN:OD1	1.98	0.64
1:A:1193:LYS:HE2	1:B:1578:CYS:CB	2.28	0.64
1:B:1299:LEU:C	1:B:1300:PHE:HD1	2.06	0.64
1:A:1244:GLU:OE2	1:A:1246:ARG:NH2	2.30	0.63
1:A:1621:GLN:NE2	6:A:1840:HOH:O	2.20	0.63
1:A:1190:LEU:HD13	1:A:1196:ALA:HB2	1.79	0.63
1:A:1254:ASP:OD1	1:A:1254:ASP:N	2.23	0.63
1:B:1244:GLU:OE1	1:B:1246:ARG:NH1	2.31	0.63
1:B:1353:PHE:CZ	1:B:1354:MET:HE3	2.34	0.63
1:A:1260:THR:OG1	1:A:1262:THR:CG2	2.47	0.62
1:A:1174:GLU:OE2	1:A:1174:GLU:CA	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:LEU:HB2	1:B:1300:PHE:CE1	2.35	0.62
1:A:1255:GLU:HG2	1:A:1264:GLN:OE1	1.99	0.61
1:A:1607:ARG:HG2	1:A:1613:LEU:HD21	1.82	0.61
1:B:1607:ARG:HG2	1:B:1613:LEU:HD21	1.84	0.60
1:B:1586:LEU:N	1:B:1586:LEU:CD2	2.64	0.60
1:B:1570:GLU:HG3	1:B:1571:PRO:HD2	1.82	0.60
1:B:1360:GLY:O	1:B:1488:LEU:HD13	2.02	0.59
1:A:1224:LEU:N	1:A:1224:LEU:HD12	2.16	0.59
1:B:1175:LYS:HG3	1:B:1176:LEU:H	1.66	0.59
1:A:1286:SER:HA	1:A:1289:GLN:HG2	1.84	0.59
1:B:1251:GLN:HE22	1:B:1256:ASN:C	2.10	0.59
1:B:1566:ARG:NH2	1:B:1570:GLU:O	2.35	0.59
1:B:1295:GLU:OE1	1:B:1295:GLU:HA	2.02	0.59
1:A:1193:LYS:HE2	1:B:1578:CYS:HA	1.85	0.58
1:A:1202:LEU:HD13	1:A:1353:PHE:CG	2.39	0.58
1:A:1411:PHE:HD2	1:A:1471:TRP:CD1	2.22	0.58
1:A:1530:PRO:O	1:A:1534:LYS:HG3	2.04	0.58
1:A:1191:GLU:HG2	1:A:1192:SER:H	1.68	0.57
1:B:1381:LYS:HE3	1:B:1480:ASN:OD1	2.05	0.57
1:A:1193:LYS:NZ	1:B:1578:CYS:HB2	2.19	0.57
1:B:1548:GLN:NE2	1:B:1552:GLU:OE2	2.38	0.57
1:B:1202:LEU:HD13	1:B:1353:PHE:CG	2.39	0.57
1:A:1225:ASN:O	1:A:1228:LEU:HD12	2.05	0.57
1:A:1293:GLN:O	1:A:1297:GLU:HG2	2.05	0.56
1:A:1296:LEU:HD23	1:A:1299:LEU:CD1	2.35	0.56
1:B:1253:SER:OG	1:B:1254:ASP:N	2.38	0.56
1:B:1192:SER:HB2	1:B:1195:ASP:OD1	2.06	0.56
1:A:1570:GLU:HG3	1:A:1571:PRO:HD2	1.87	0.55
1:A:1607:ARG:O	1:A:1610:SER:N	2.39	0.55
1:B:1293:GLN:NE2	1:B:1297:GLU:OE2	2.39	0.55
1:A:1228:LEU:HA	1:A:1233:THR:HG21	1.87	0.55
1:B:1174:GLU:O	1:B:1175:LYS:O	2.24	0.55
1:A:1379:TYR:O	1:A:1479:ASN:HA	2.06	0.55
1:B:1328:PHE:CD1	1:B:1328:PHE:C	2.85	0.55
1:B:1258:ASP:OD2	1:B:1263:ARG:CG	2.55	0.54
1:B:1530:PRO:O	1:B:1534:LYS:HG3	2.08	0.54
1:A:1244:GLU:OE2	1:A:1246:ARG:CZ	2.55	0.54
1:A:1254:ASP:HB2	1:A:1441:LEU:HD12	1.89	0.54
1:A:1239:GLY:O	1:A:1276:THR:HB	2.07	0.54
1:A:1548:GLN:NE2	1:A:1552:GLU:OE2	2.41	0.54
1:B:1566:ARG:HA	1:B:1570:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1199:PRO:O	1:B:1203:GLN:HG2	2.07	0.53
1:B:1181:LEU:C	1:B:1183:PRO:HD3	2.33	0.53
1:A:1190:LEU:HD22	1:A:1195:ASP:HB2	1.91	0.53
1:B:1255:GLU:HG2	1:B:1264:GLN:HE22	1.73	0.53
1:A:1193:LYS:CD	1:A:1221:SER:O	2.57	0.53
1:A:1300:PHE:O	1:A:1301:GLN:CG	2.57	0.53
1:B:1403:ILE:CG2	1:B:1479:ASN:C	2.79	0.53
1:A:1266:TRP:HB2	1:A:1267:PRO:HD3	1.91	0.52
1:A:1566:ARG:HA	1:A:1570:GLU:OE1	2.09	0.52
1:A:1228:LEU:O	1:A:1233:THR:CB	2.57	0.52
1:A:1328:PHE:CD1	1:A:1328:PHE:C	2.87	0.52
1:B:1239:GLY:O	1:B:1276:THR:HB	2.09	0.52
1:A:1224:LEU:CD1	1:A:1224:LEU:N	2.72	0.52
1:A:1609:ARG:O	1:A:1609:ARG:CG	2.58	0.52
1:A:1297:GLU:O	1:A:1300:PHE:N	2.44	0.51
1:A:1410:TRP:NE1	1:A:1456:GLN:OE1	2.38	0.51
1:B:1564:GLN:O	1:B:1621:GLN:HA	2.09	0.51
1:A:1267:PRO:HG3	1:A:1430:VAL:CG2	2.40	0.51
1:B:1222:LEU:HB2	1:B:1224:LEU:CD1	2.41	0.51
1:B:1251:GLN:NE2	1:B:1255:GLU:O	2.37	0.50
1:B:1372:GLY:O	2:D:27:M3L:HM13	2.11	0.50
1:B:1403:ILE:O	1:B:1403:ILE:HG13	2.04	0.50
1:A:1366:VAL:HG11	1:A:1370:ILE:HD11	1.94	0.50
1:B:1224:LEU:HD12	1:B:1224:LEU:H	1.75	0.50
1:A:1234:LEU:HD13	1:A:1378:LEU:HD21	1.94	0.50
1:B:1251:GLN:HE22	1:B:1257:TRP:N	2.09	0.50
1:B:1413:VAL:HG12	1:B:1414:HIS:N	2.27	0.49
1:B:1258:ASP:OD2	1:B:1263:ARG:HG3	2.12	0.49
1:A:1384:GLY:HA2	1:A:1473:GLN:HE21	1.78	0.49
1:B:1612:GLY:C	1:B:1614:GLN:OE1	2.56	0.49
1:B:1218:LEU:HD22	1:B:1461:LEU:HD13	1.94	0.49
1:A:1564:GLN:O	1:A:1621:GLN:HA	2.12	0.49
1:A:1575:CYS:C	1:A:1577:GLU:H	2.21	0.49
1:A:1250:GLN:OE1	1:A:1324:HIS:ND1	2.35	0.49
1:A:1585:ILE:C	1:A:1586:LEU:HD23	2.38	0.48
1:A:1588:VAL:HA	1:A:1599:LEU:O	2.12	0.48
1:B:1575:CYS:HB3	1:B:1579:ASP:N	2.27	0.48
1:A:1232:LYS:O	1:A:1236:GLU:HG2	2.13	0.48
1:A:1243:VAL:HG23	1:A:1244:GLU:O	2.12	0.48
1:B:1488:LEU:HD12	1:B:1488:LEU:N	2.27	0.48
1:B:1541:LEU:O	1:B:1545:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1195:ASP:O	1:B:1198:SER:HB3	2.14	0.48
1:B:1488:LEU:N	1:B:1488:LEU:CD1	2.76	0.48
1:A:1193:LYS:HE2	1:B:1578:CYS:CA	2.43	0.48
1:A:1226:LEU:O	1:A:1227:GLY:C	2.56	0.48
1:B:1425:CYS:HB3	1:B:1430:VAL:O	2.14	0.48
1:A:1195:ASP:O	1:A:1198:SER:HB3	2.13	0.48
1:B:1586:LEU:HB2	1:B:1619:LEU:HB2	1.96	0.48
1:B:1488:LEU:CD2	1:B:1525:VAL:HG11	2.44	0.48
1:B:1403:ILE:HG21	1:B:1479:ASN:HB2	1.96	0.47
1:A:1289:GLN:HG3	1:A:1290:GLU:H	1.79	0.47
1:A:1541:LEU:O	1:A:1545:LYS:HG3	2.14	0.47
1:B:1243:VAL:HG23	1:B:1332:ILE:HG12	1.96	0.47
1:A:1260:THR:OG1	1:A:1262:THR:HG23	2.14	0.47
1:A:1419:GLU:H	1:A:1419:GLU:HG2	1.48	0.47
1:B:1234:LEU:HD13	1:B:1378:LEU:HD21	1.96	0.47
1:A:1494:GLN:O	1:A:1498:GLU:HG3	2.15	0.47
1:A:1297:GLU:O	1:A:1298:VAL:C	2.58	0.47
1:B:1379:TYR:O	1:B:1479:ASN:HA	2.14	0.47
1:A:1297:GLU:O	1:A:1301:GLN:N	2.48	0.47
1:A:1607:ARG:O	1:A:1610:SER:O	2.31	0.47
6:A:1813:HOH:O	2:C:27:M3L:HM32	2.15	0.47
2:C:24:ALA:O	2:C:25:ALA:C	2.55	0.47
1:A:1196:ALA:HA	1:A:1201:LEU:HD22	1.96	0.47
1:B:1224:LEU:N	1:B:1224:LEU:CD1	2.75	0.47
1:B:1503:ASN:HB3	1:B:1508:VAL:O	2.15	0.47
2:D:26:ARG:CG	2:D:27:M3L:N	2.78	0.47
1:A:1250:GLN:HB3	1:A:1324:HIS:HB3	1.97	0.47
1:B:1192:SER:HB2	1:B:1195:ASP:CG	2.40	0.46
1:B:1371:LEU:HA	1:B:1375:THR:OG1	2.16	0.46
1:A:1578:CYS:SG	1:A:1580:VAL:HG12	2.55	0.46
1:B:1299:LEU:HB2	1:B:1300:PHE:CD1	2.50	0.46
1:B:1588:VAL:HA	1:B:1599:LEU:O	2.14	0.46
1:A:1381:LYS:HE3	1:A:1480:ASN:OD1	2.16	0.46
1:B:1188:ILE:HD12	1:B:1213:THR:CG2	2.46	0.46
1:B:1494:GLN:O	1:B:1498:GLU:HG3	2.16	0.46
1:B:1419:GLU:H	1:B:1419:GLU:HG2	1.49	0.46
1:B:1528:SER:HA	1:B:1637:ALA:O	2.16	0.46
1:B:1250:GLN:OE1	1:B:1324:HIS:ND1	2.43	0.46
1:B:1392:GLU:OE1	2:D:27:M3L:HM23	2.16	0.46
1:A:1226:LEU:O	1:A:1228:LEU:N	2.49	0.46
1:B:1175:LYS:CG	1:B:1176:LEU:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1403:ILE:CG2	1:B:1479:ASN:HB2	2.46	0.46
1:A:1226:LEU:O	1:A:1229:PHE:N	2.39	0.46
6:A:1813:HOH:O	2:C:27:M3L:CM3	2.64	0.46
1:B:1178:ARG:O	1:B:1181:LEU:N	2.46	0.46
1:A:1300:PHE:O	1:A:1301:GLN:HG3	2.16	0.46
1:A:1425:CYS:HB3	1:A:1430:VAL:O	2.16	0.45
1:B:1586:LEU:N	1:B:1586:LEU:HD22	2.30	0.45
1:A:1510:SER:HB2	6:A:1808:HOH:O	2.16	0.45
1:A:1538:PHE:O	1:A:1542:GLN:HG2	2.17	0.45
1:B:1175:LYS:CG	1:B:1176:LEU:N	2.80	0.45
1:B:1361:ASN:O	1:B:1362:MET:C	2.59	0.45
1:A:1411:PHE:CD2	1:A:1471:TRP:NE1	2.85	0.45
1:A:1192:SER:OG	1:A:1194:ARG:HG2	2.17	0.45
1:B:1258:ASP:OD2	1:B:1263:ARG:HG2	2.16	0.45
1:B:1242:THR:HG23	1:B:1243:VAL:N	2.31	0.45
1:B:1341:LYS:HE2	1:B:1341:LYS:HB2	1.72	0.45
1:B:1436:SER:HB3	2:D:32:THR:HG21	1.99	0.44
1:B:1538:PHE:O	1:B:1542:GLN:HG2	2.18	0.44
1:B:1613:LEU:N	1:B:1614:GLN:OE1	2.50	0.44
1:B:1366:VAL:HG11	1:B:1370:ILE:HD11	1.99	0.44
1:B:1394:ASN:O	1:B:1496:ALA:HA	2.17	0.44
1:B:1578:CYS:O	1:B:1579:ASP:HB2	2.17	0.44
2:D:26:ARG:HG3	2:D:27:M3L:N	2.31	0.44
1:A:1251:GLN:HE22	1:A:1256:ASN:CA	2.08	0.44
1:A:1502:TRP:CZ2	1:A:1506:LYS:HE3	2.53	0.44
1:B:1504:GLU:HG3	1:B:1505:VAL:N	2.31	0.44
1:A:1269:GLU:CD	2:C:32:THR:HG21	2.42	0.44
1:A:1427:ARG:HH11	1:A:1427:ARG:CG	2.30	0.44
1:B:1178:ARG:O	1:B:1181:LEU:HB2	2.17	0.44
1:A:1293:GLN:C	1:A:1295:GLU:H	2.26	0.44
1:A:1633:ALA:C	1:B:1259:LEU:HD21	2.43	0.44
1:B:1298:VAL:O	1:B:1298:VAL:CG1	2.63	0.44
1:B:1410:TRP:NE1	1:B:1456:GLN:OE1	2.46	0.44
1:A:1300:PHE:O	1:A:1301:GLN:CD	2.57	0.43
1:A:1341:LYS:HB2	1:A:1341:LYS:HE2	1.70	0.43
1:A:1536:ILE:O	1:A:1540:LEU:HG	2.18	0.43
1:B:1399:VAL:O	1:B:1399:VAL:HG12	2.17	0.43
1:A:1614:GLN:H	1:A:1614:GLN:CD	2.10	0.43
1:B:1188:ILE:HD11	1:B:1204:PHE:CD2	2.51	0.43
1:B:1207:ASP:HA	1:B:1208:PRO:HD3	1.88	0.43
1:B:1502:TRP:CZ2	1:B:1506:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1575:CYS:C	1:A:1577:GLU:N	2.77	0.43
1:B:1597:THR:CG2	1:B:1598:TYR:N	2.58	0.43
1:A:1298:VAL:HG23	1:A:1299:LEU:N	2.32	0.43
1:A:1607:ARG:O	1:A:1610:SER:C	2.62	0.43
1:A:1381:LYS:HB3	1:A:1385:SER:HB2	2.00	0.43
1:A:1422:SER:HA	1:A:1432:TYR:CD1	2.54	0.43
1:B:1563:TYR:CE1	1:B:1623:ARG:HG3	2.54	0.43
1:B:1275:THR:HB	1:B:1276:THR:H	1.47	0.43
1:A:1282:GLN:OE1	1:A:1282:GLN:HA	2.19	0.42
1:B:1267:PRO:HG3	1:B:1430:VAL:CG2	2.49	0.42
1:B:1457:ARG:HB3	1:B:1458:PRO:HD2	2.01	0.42
1:A:1160:LEU:CD1	1:A:1497:LEU:HB3	2.27	0.42
1:A:1523:ARG:O	1:B:1258:ASP:HB2	2.20	0.42
1:B:1431:ASP:OD2	1:B:1434:THR:OG1	2.23	0.42
1:A:1193:LYS:CE	1:B:1578:CYS:HB2	2.49	0.42
1:A:1193:LYS:HD3	1:A:1221:SER:O	2.18	0.42
1:A:1286:SER:O	1:A:1289:GLN:CG	2.67	0.42
1:A:1504:GLU:HG3	1:A:1505:VAL:N	2.32	0.42
1:A:1272:ARG:CG	1:A:1273:SER:N	2.81	0.42
1:A:1371:LEU:HA	1:A:1375:THR:OG1	2.20	0.42
1:B:1484:ASN:OD1	2:D:27:M3L:HM22	2.18	0.42
1:B:1609:ARG:O	1:B:1609:ARG:CG	2.65	0.42
1:A:1503:ASN:HB3	1:A:1508:VAL:O	2.20	0.42
1:A:1528:SER:HA	1:A:1637:ALA:O	2.20	0.42
1:A:1341:LYS:O	1:A:1345:GLN:HG3	2.20	0.42
1:B:1519:TRP:CD1	1:B:1583:PHE:CZ	3.08	0.42
1:B:1224:LEU:CD1	1:B:1224:LEU:H	2.32	0.41
1:A:1226:LEU:C	1:A:1228:LEU:N	2.78	0.41
1:A:1563:TYR:CE1	1:A:1623:ARG:HG3	2.55	0.41
1:B:1399:VAL:HG11	1:B:1483:TRP:CZ2	2.55	0.41
1:A:1190:LEU:HA	1:A:1190:LEU:HD23	1.84	0.41
1:A:1341:LYS:CG	1:A:1345:GLN:OE1	2.68	0.41
1:B:1293:GLN:O	1:B:1297:GLU:HG2	2.20	0.41
1:A:1362:MET:HG3	1:A:1488:LEU:HD23	2.02	0.41
1:A:1427:ARG:NH1	1:A:1427:ARG:HG3	2.35	0.41
1:A:1526:LYS:HD3	1:A:1526:LYS:HA	1.96	0.41
1:B:1585:ILE:C	1:B:1586:LEU:HD22	2.45	0.41
1:A:1286:SER:O	1:A:1289:GLN:HG2	2.21	0.41
1:A:1457:ARG:O	1:A:1460:ASP:HB2	2.20	0.41
1:A:1394:ASN:O	1:A:1496:ALA:HA	2.20	0.41
1:A:1519:TRP:CD2	1:A:1540:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1167:LYS:HG2	6:B:1831:HOH:O	2.21	0.41
1:B:1422:SER:HA	1:B:1432:TYR:CD1	2.56	0.41
1:B:1519:TRP:CD2	1:B:1540:LEU:HD22	2.56	0.41
1:A:1193:LYS:HE2	1:B:1578:CYS:HB2	2.00	0.41
1:B:1299:LEU:HB2	1:B:1300:PHE:HE1	1.84	0.41
1:B:1519:TRP:CE2	1:B:1540:LEU:HD22	2.56	0.41
1:B:1536:ILE:O	1:B:1540:LEU:HG	2.21	0.41
1:A:1192:SER:HG	1:A:1194:ARG:HG2	1.86	0.41
1:A:1361:ASN:O	1:A:1362:MET:C	2.63	0.41
1:A:1399:VAL:HG11	1:A:1483:TRP:CZ2	2.56	0.41
1:A:1497:LEU:HD12	1:A:1497:LEU:HA	1.85	0.41
1:B:1266:TRP:HB2	1:B:1267:PRO:HD3	2.02	0.41
1:A:1413:VAL:HG12	1:A:1414:HIS:N	2.35	0.40
1:B:1341:LYS:O	1:B:1345:GLN:HG3	2.21	0.40
1:A:1359:THR:HG23	1:B:1429:GLY:O	2.20	0.40
1:A:1566:ARG:HG3	1:A:1622:TYR:CZ	2.56	0.40
1:A:1298:VAL:O	1:A:1299:LEU:C	2.64	0.40
1:B:1588:VAL:HG13	1:B:1599:LEU:O	2.21	0.40
1:B:1270:SER:N	2:D:32:THR:OG1	2.47	0.40
1:B:1242:THR:CG2	1:B:1243:VAL:N	2.82	0.40
1:B:1586:LEU:N	1:B:1586:LEU:HD23	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:LYS:O	1:A:1339:ARG:NH2[3_544]	2.04	0.16

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	449/486 (92%)	425 (95%)	23 (5%)	1 (0%)	43	62
1	B	443/486 (91%)	424 (96%)	18 (4%)	1 (0%)	43	62
2	C	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
2	D	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
All	All	908/994 (91%)	862 (95%)	44 (5%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1175	LYS
1	A	1227	GLY

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	404/424 (95%)	364 (90%)	40 (10%)	7	15
1	B	400/424 (94%)	359 (90%)	41 (10%)	7	13
2	C	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	D	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	812/856 (95%)	728 (90%)	84 (10%)	7	13

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1157	GLU
1	A	1173	GLU
1	A	1174	GLU
1	A	1175	LYS
1	A	1188	ILE
1	A	1191	GLU
1	A	1192	SER
1	A	1200	VAL
1	A	1218	LEU

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Mol	Chain	Res	Type
1	A	1232	LYS
1	A	1242	THR
1	A	1243	VAL
1	A	1262	THR
1	A	1263	ARG
1	A	1273	SER
1	A	1275	THR
1	A	1282	GLN
1	A	1287	SER
1	A	1292	LEU
1	A	1300	PHE
1	A	1301	GLN
1	A	1325	ILE
1	A	1327	LYS
1	A	1341	LYS
1	A	1387	THR
1	A	1399	VAL
1	A	1419	GLU
1	A	1427	ARG
1	A	1497	LEU
1	A	1504	GLU
1	A	1510	SER
1	A	1523	ARG
1	A	1528	SER
1	A	1549	VAL
1	A	1552	GLU
1	A	1560	LYS
1	A	1608	ARG
1	A	1609	ARG
1	A	1614	GLN
1	A	1617	VAL
1	B	1157	GLU
1	B	1179	GLU
1	B	1190	LEU
1	B	1193	LYS
1	B	1214	VAL
1	B	1221	SER
1	B	1223	ARG
1	B	1224	LEU
1	B	1238	SER
1	B	1242	THR
1	B	1246	ARG

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Mol	Chain	Res	Type
1	B	1251	GLN
1	B	1263	ARG
1	B	1273	SER
1	B	1275	THR
1	B	1282	GLN
1	B	1294	GLU
1	B	1295	GLU
1	B	1296	LEU
1	B	1298	VAL
1	B	1300	PHE
1	B	1325	ILE
1	B	1327	LYS
1	B	1339	ARG
1	B	1341	LYS
1	B	1387	THR
1	B	1399	VAL
1	B	1403	ILE
1	B	1419	GLU
1	B	1427	ARG
1	B	1497	LEU
1	B	1504	GLU
1	B	1510	SER
1	B	1523	ARG
1	B	1528	SER
1	B	1549	VAL
1	B	1560	LYS
1	B	1586	LEU
1	B	1609	ARG
1	B	1614	GLN
1	B	1617	VAL
2	C	26	ARG
2	C	32	THR
2	D	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1182	ASN
1	A	1251	GLN
1	A	1256	ASN
1	A	1416	HIS
1	A	1621	GLN

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Mol	Chain	Res	Type
1	B	1182	ASN
1	B	1210	ASN
1	B	1251	GLN
1	B	1264	GLN
1	B	1289	GLN
1	B	1394	ASN
1	B	1416	HIS
1	B	1516	HIS
1	B	1576	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	M3L	C	27	2	10,11,12	1.65	3 (30%)	9,14,16	0.65	0
2	M3L	D	27	2	10,11,12	0.88	0	9,14,16	0.29	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	M3L	C	27	2	-	4/9/10/12	-
2	M3L	D	27	2	-	5/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	27	M3L	CM2-NZ	-3.10	1.41	1.50
2	C	27	M3L	CE-NZ	-2.61	1.43	1.51
2	C	27	M3L	CB-CA	-2.34	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	27	M3L	C-CA-CB-CG
2	D	27	M3L	O-C-CA-CB
2	C	27	M3L	CE-CD-CG-CB
2	C	27	M3L	CA-CB-CG-CD
2	D	27	M3L	N-CA-CB-CG
2	D	27	M3L	CD-CE-NZ-CM1
2	D	27	M3L	CD-CE-NZ-CM3
2	C	27	M3L	CD-CE-NZ-CM2
2	C	27	M3L	CD-CE-NZ-CM1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	27	M3L	2	0
2	D	27	M3L	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OGA	B	1703	3	9,9,9	1.69	1 (11%)	8,11,11	2.19	2 (25%)
5	OGA	A	1703	3	9,9,9	2.16	1 (11%)	8,11,11	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OGA	B	1703	3	-	1/8/9/9	-
5	OGA	A	1703	3	-	0/8/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1703	OGA	C2-C1	-5.62	1.47	1.54
5	B	1703	OGA	C2-C1	4.15	1.59	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1703	OGA	O2'-C2-C1	4.65	127.46	121.36
5	B	1703	OGA	O2-C1-O1	-3.00	116.75	123.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1703	OGA	C5-C4-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	455/486 (93%)	0.24	20 (4%) 39 35	24, 53, 94, 122	0
1	B	451/486 (92%)	0.25	22 (4%) 35 31	36, 54, 92, 119	0
2	C	10/11 (90%)	2.52	4 (40%) 1 0	58, 81, 109, 109	0
2	D	10/11 (90%)	2.24	6 (60%) 0 0	53, 76, 115, 118	0
All	All	926/994 (93%)	0.29	52 (5%) 30 27	24, 54, 95, 122	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1174	GLU	7.7
1	B	1299	LEU	7.2
1	B	1252	PRO	6.9
1	B	1253	SER	6.6
1	A	1171	ASN	5.4
1	B	1300	PHE	5.4
1	B	1298	VAL	5.2
1	A	1299	LEU	5.2
2	C	28	SER	5.0
2	C	24	ALA	4.8
1	A	1597	THR	4.5
1	B	1254	ASP	4.2
1	A	1172	THR	4.2
2	C	34	GLY	4.0
2	C	25	ALA	3.6
1	A	1294	GLU	3.6
1	A	1590	SER	3.4
1	B	1270	SER	3.4
1	B	1271	SER	3.4
1	A	1300	PHE	3.4
1	A	1228	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	25	ALA	3.2
1	B	1575	CYS	3.2
1	B	1290	GLU	3.2
1	A	1546	HIS	3.1
1	B	1597	THR	3.1
1	B	1590	SER	3.1
1	A	1169	LYS	3.0
1	B	1174	GLU	3.0
2	D	24	ALA	3.0
1	B	1568	LYS	2.9
1	A	1225	ASN	2.8
1	B	1638	PRO	2.7
1	A	1638	PRO	2.7
1	B	1170	ILE	2.6
1	B	1294	GLU	2.6
2	D	28	SER	2.6
2	D	29	ALA	2.5
1	A	1189	TYR	2.4
1	A	1298	VAL	2.4
1	A	1323	HIS	2.4
1	A	1157	GLU	2.4
2	D	34	GLY	2.3
1	B	1189	TYR	2.3
1	B	1222	LEU	2.3
1	A	1175	LYS	2.3
1	B	1323	HIS	2.3
1	B	1157	GLU	2.2
1	A	1240	GLU	2.1
2	D	31	ALA	2.1
1	B	1488	LEU	2.1
1	A	1254	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	M3L	C	27	12/13	0.89	0.16	44,62,69,72	0
2	M3L	D	27	12/13	0.89	0.18	48,66,75,78	0

6.3 Carbohydrates [i](#)

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
5	OGA	B	1703	10/10	0.78	0.24	20,20,20,20	0
5	OGA	A	1703	10/10	0.81	0.20	20,20,20,20	0
4	ZN	A	1702	1/1	0.94	0.06	56,56,56,56	0
4	ZN	B	1702	1/1	0.95	0.08	57,57,57,57	0
3	NI	A	1701	1/1	0.98	0.04	34,34,34,34	0
3	NI	B	1701	1/1	0.98	0.06	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.