Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID	:	4EZH
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
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:

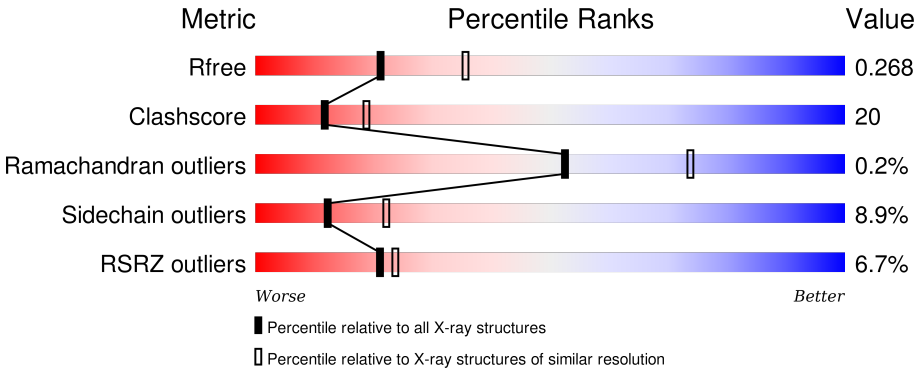
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (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 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 <=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	7% 59% 30% 5% 6%
1	B	486	5% 58% 31% • 7%
2	C	11	18% 55% 36% 9%
2	D	11	9% 64% 27% 9%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OGA	B	1703	-	-	-	X

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 3668 2331 8 635 675 19	0	0	0
1	B	451	Total C N O S 3627 2313 629 666 19	0	0	0

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 (three-letter code: NI) (formula: Ni).

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

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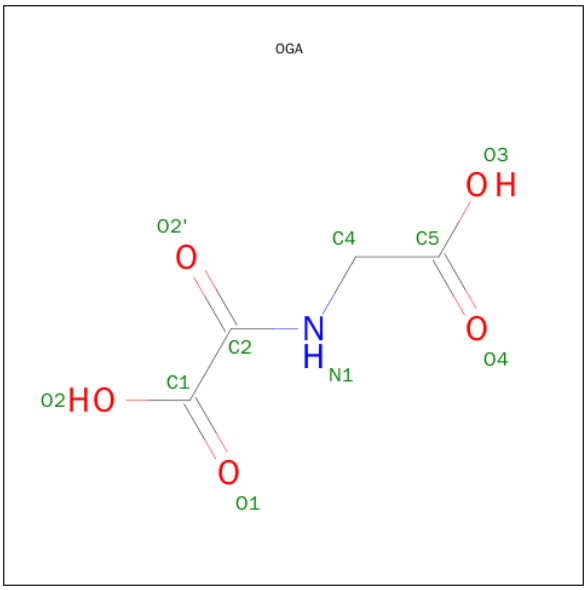
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



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.

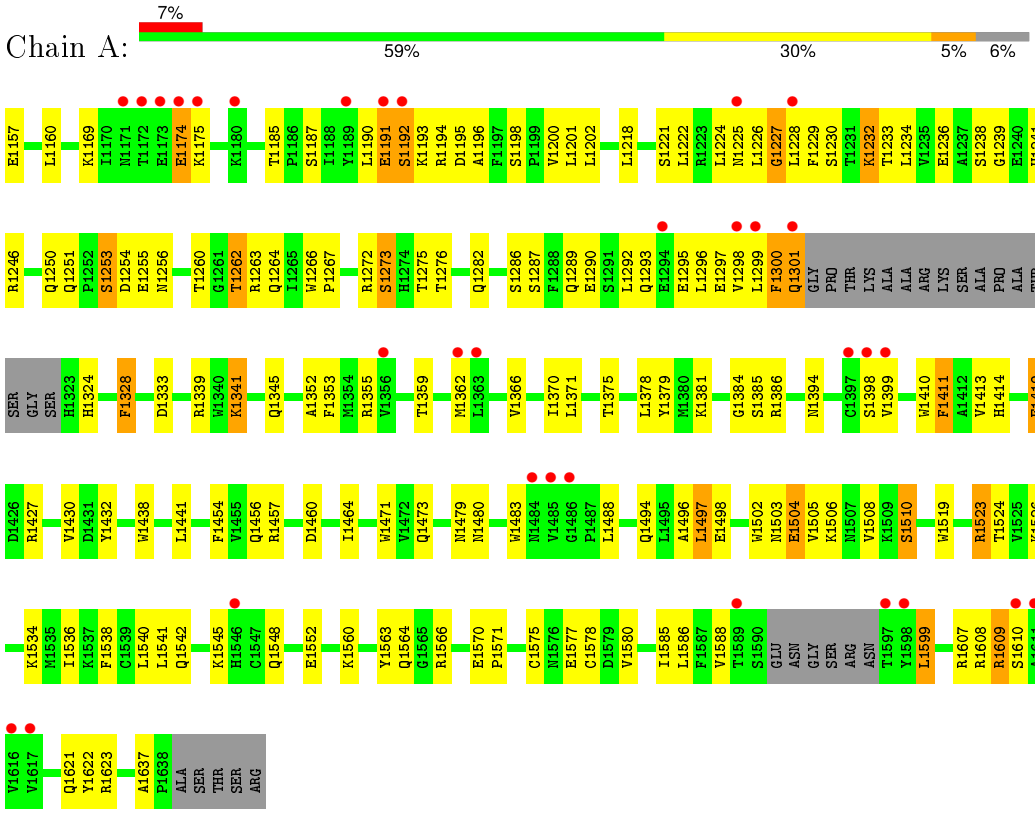
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	39	Total O 39 39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

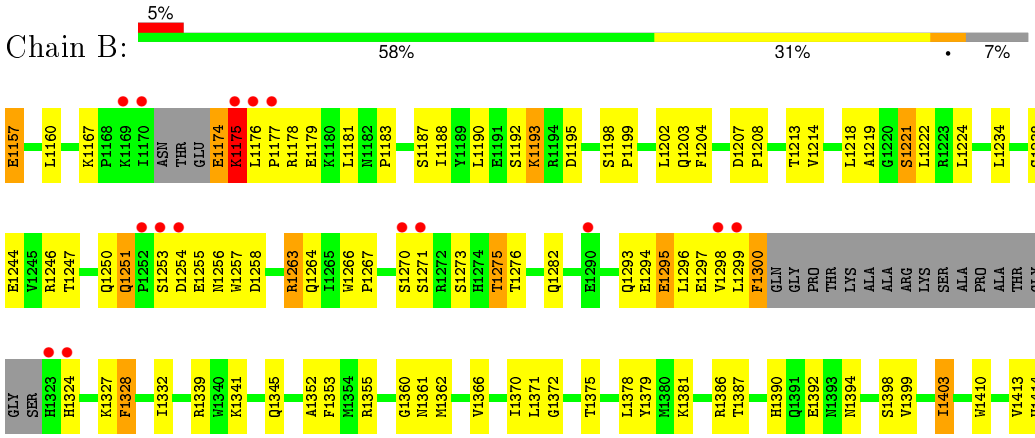
- Molecule 1: Lysine-specific demethylase 6B

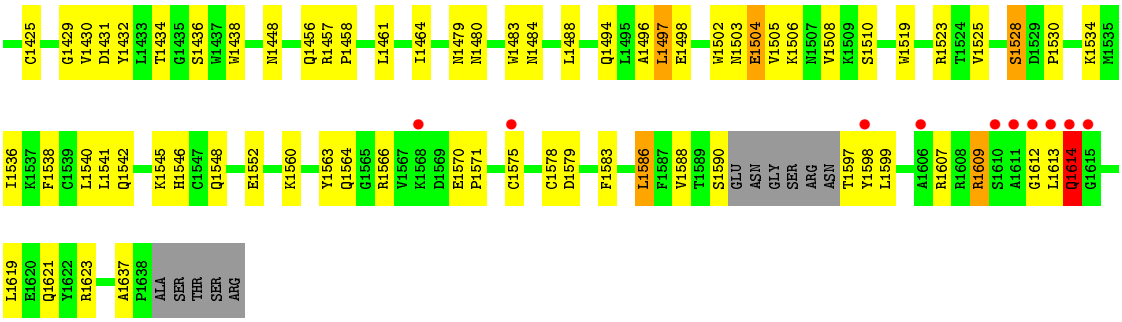
Chain A:



- Molecule 1: Lysine-specific demethylase 6B

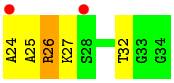
Chain B:





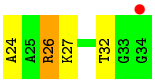
- Molecule 2: SYNTHESIZED methylation peptide

Chain C:



- Molecule 2: SYNTHESIZED methylation peptide

Chain D:



4 Data and refinement statistics (i)

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 40.16 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-2.52) 87.6 (40.16-2.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.213 , 0.254 0.226 , 0.268	Depositor DCC
R_{free} test set	2113 reflections (6.01%)	DCC
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Outliers	4 of 41826 reflections (0.010%)	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 50.27 % 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 6.6257e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NI, ZN, M3L, OGA

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	0.63	4/3755 (0.1%)	0.64	1/5110 (0.0%)
1	B	0.63	0/3721	0.63	1/5062 (0.0%)
2	C	1.47	0/59	1.18	0/79
2	D	0.38	0/59	0.68	0/79
All	All	0.64	4/7594 (0.1%)	0.64	2/10330 (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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1411	PHE	CE1-CZ	-5.76	1.26	1.37
1	A	1411	PHE	CG-CD1	-5.67	1.30	1.38
1	A	1411	PHE	CE2-CZ	-5.65	1.26	1.37
1	A	1411	PHE	CG-CD2	-5.40	1.30	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1614	GLN	CA-CB-CG	5.37	125.21	113.40
1	B	1614	GLN	CA-CB-CG	5.03	124.47	113.40

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	144	1
1	B	3627	0	3551	151	0
2	C	71	0	75	6	0
2	D	71	0	75	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	7287	297	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 20.

All (297) 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:HA	1:B:1157:GLU:OE1	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:B:1219:ALA:HA	1:B:1224:LEU:HD13	1.37	1.06
1:A:1251:GLN:HE22	1:A:1256:ASN:HA	1.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:1300:PHE:CD1	2.39	0.85
1:B:1193:LYS:HG3	1:B:1221:SER:O	1.77	0.84
1:A:1251:GLN:NE2	1:A:1256:ASN:HA	1.93	0.84
1:A:1222:LEU:HB2	1:A:1224:LEU:HD11	1.60	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:B:1251:GLN:HE21	1:B:1256:ASN:HA	1.44	0.82
1:A:1253:SER:HA	1:A:1473:GLN:OE1	1.79	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:HD1	1:A:1300:PHE:N	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:A:1191:GLU:HG2	1:A:1192:SER:N	2.05	0.72
1:B:1222:LEU:HB2	1:B:1224:LEU:HD11	1.71	0.71
1:B:1193:LYS:N	1:B:1193:LYS:CD	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:1289:GLN:HG3	1:A:1290:GLU:N	2.07	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: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:B:1403:ILE:HG23	1:B:1479:ASN:C	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1590:SER:HA	1:B:1597:THR:O	1.94	0.67
1:A:1295:GLU:O	1:A:1299:LEU:HG	1.94	0.67
1:A:1193:LYS:CG	1:A:1221:SER:O	2.42	0.67
2:D:26:ARG:HH11	2:D:26:ARG:HG2	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: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
2:D:26:ARG:CG	2:D:26:ARG:HH11	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: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:N	1:A:1254:ASP:OD1	2.23	0.63
1:B:1244:GLU:OE1	1:B:1246:ARG:NH1	2.31	0.63
1:A:1260:THR:OG1	1:A:1262:THR:CG2	2.47	0.62
1:A:1174:GLU:CA	1:A:1174:GLU:OE2	2.34	0.62
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:CD2	1:B:1586:LEU:N	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:HD12	1:A:1224:LEU:N	2.16	0.59
1:B:1175:LYS:HG3	1:B:1176:LEU:H	1.66	0.59
1:A:1612:GLY:C	1:A:1614:GLN:OE1	2.40	0.59
1:A:1286:SER:HA	1:A:1289:GLN:HG2	1.84	0.59
1:B:1299:LEU:C	1:B:1300:PHE:HD1	2.06	0.59
1:B:1566:ARG:NH2	1:B:1570:GLU:O	2.35	0.59
1:B:1295:GLU:HA	1:B:1295:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1251:GLN:HE22	1:B:1256:ASN:C	2.10	0.54
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
1:B:1199:PRO:O	1:B:1203:GLN:HG2	2.07	0.53
1:B:1255:GLU:HG2	1:B:1264:GLN:HE22	1.73	0.53
1:A:1190:LEU:HD22	1:A:1195:ASP:HB2	1.91	0.53
1:A:1300:PHE:O	1:A:1301:GLN:CG	2.57	0.53
1:A:1193:LYS:CD	1:A:1221:SER:O	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1403:ILE:O	1:B:1403:ILE:HG13	2.04	0.50
1:B:1372:GLY:O	2:D:27:M3L:HM13	2.11	0.50
1:B:1328:PHE:C	1:B:1328:PHE:CD1	2.85	0.50
1:A:1185:THR:HG1	1:A:1454:PHE:HD2	1.58	0.50
1:B:1224:LEU:HD12	1:B:1224:LEU:H	1.75	0.50
1:A:1366:VAL:HG11	1:A:1370:ILE:HD11	1.94	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: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:B:1181:LEU:C	1:B:1183:PRO:HD3	2.33	0.49
1:A:1250:GLN:OE1	1:A:1324:HIS:ND1	2.35	0.49
1:B:1575:CYS:HB3	1:B:1579:ASP:N	2.27	0.48
1:A:1588:VAL:HA	1:A:1599:LEU:O	2.12	0.48
1:A:1232:LYS:O	1:A:1236:GLU:HG2	2.13	0.48
1:B:1541:LEU:O	1:B:1545:LYS:HG3	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:1488:LEU:CD1	1:B:1488:LEU:N	2.76	0.48
1:B:1195:ASP:O	1:B:1198:SER:HB3	2.14	0.48
1:A:1193:LYS:HE2	1:B:1578:CYS:CA	2.43	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:A:1328:PHE:CD1	1:A:1328:PHE:C	2.87	0.47
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:1298:VAL:O	1:B:1298:VAL:CG1	2.63	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:B:1234:LEU:HD13	1:B:1378:LEU:HD21	1.96	0.47
1:A:1419:GLU:HG2	1:A:1419:GLU:H	1.48	0.47
1:A:1494:GLN:O	1:A:1498:GLU:HG3	2.15	0.47
1:B:1379:TYR:O	1:B:1479:ASN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1297:GLU:O	1:A:1301:GLN:N	2.48	0.47
6:A:1813:HOH:O	2:C:27:M3L:HM32	2.15	0.47
1:A:1607:ARG:O	1:A:1610:SER:O	2.31	0.47
1:B:1224:LEU:N	1:B:1224:LEU:CD1	2.75	0.47
2:D:26:ARG:CG	2:D:27:M3L:N	2.78	0.47
1:A:1196:ALA:HA	1:A:1201:LEU:HD22	1.96	0.47
1:B:1503:ASN:HB3	1:B:1508:VAL:O	2.15	0.47
1:A:1250:GLN:HB3	1:A:1324:HIS:HB3	1.97	0.47
1:B:1371:LEU:HA	1:B:1375:THR:OG1	2.16	0.46
1:B:1299:LEU:HB2	1:B:1300:PHE:CD1	2.50	0.46
1:A:1578:CYS:SG	1:A:1580:VAL:HG12	2.55	0.46
1:B:1588:VAL:HA	1:B:1599:LEU:O	2.14	0.46
1:B:1188:ILE:HD12	1:B:1213:THR:CG2	2.46	0.46
1:A:1381:LYS:HE3	1:A:1480:ASN:OD1	2.16	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:1392:GLU:OE1	2:D:27:M3L:HM23	2.16	0.46
1:B:1250:GLN:OE1	1:B:1324:HIS:ND1	2.43	0.46
1:B:1403:ILE:CG2	1:B:1479:ASN:HB2	2.46	0.46
1:B:1175:LYS:CG	1:B:1176:LEU:H	2.28	0.46
1:A:1226:LEU:O	1:A:1228:LEU:N	2.49	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:B:1586:LEU:HD22	1:B:1586:LEU:N	2.30	0.45
1:A:1425:CYS:HB3	1:A:1430:VAL:O	2.16	0.45
1:B:1242:THR:HG23	1:B:1243:VAL:N	2.31	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: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:1341:LYS:HE2	1:B:1341:LYS:HB2	1.72	0.45
1:B:1613:LEU:N	1:B:1614:GLN:OE1	2.50	0.44
1:B:1609:ARG:O	1:B:1609:ARG:CG	2.65	0.44
1:B:1538:PHE:O	1:B:1542:GLN:HG2	2.18	0.44
1:B:1436:SER:HB3	2:D:32:THR:HG21	1.99	0.44
1:B:1612:GLY:C	1:B:1614:GLN:OE1	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1578:CYS:O	1:B:1579:ASP:HB2	2.17	0.44
1:B:1394:ASN:O	1:B:1496:ALA:HA	2.17	0.44
1:B:1366:VAL:HG11	1:B:1370:ILE:HD11	1.99	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:1575:CYS:C	1:A:1577:GLU:H	2.21	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:1298:VAL:HG23	1:A:1299:LEU:N	2.32	0.44
1:B:1178:ARG:O	1:B:1181:LEU:HB2	2.17	0.44
1:A:1585:ILE:C	1:A:1586:LEU:HD23	2.38	0.44
1:A:1427:ARG:HH11	1:A:1427:ARG:CG	2.30	0.44
1:B:1410:TRP:NE1	1:B:1456:GLN:OE1	2.46	0.44
1:A:1536:ILE:O	1:A:1540:LEU:HG	2.18	0.43
1:A:1341:LYS:HE2	1:A:1341:LYS:HB2	1.70	0.43
1:B:1399:VAL:HG12	1:B:1399:VAL:O	2.17	0.43
1:B:1188:ILE:HD11	1:B:1204:PHE:CD2	2.51	0.43
1:B:1502:TRP:CZ2	1:B:1506:LYS:HE3	2.53	0.43
1:B:1207:ASP:HA	1:B:1208:PRO:HD3	1.88	0.43
1:B:1597:THR:CG2	1:B:1598:TYR:N	2.58	0.43
1:B:1609:ARG:HG2	1:B:1609:ARG:O	2.19	0.43
1:A:1226:LEU:O	1:A:1227:GLY:C	2.56	0.43
1:B:1403:ILE:CG2	1:B:1479:ASN:C	2.79	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:1371:LEU:O	2:C:27:M3L:N	2.52	0.42
1:B:1267:PRO:HG3	1:B:1430:VAL:CG2	2.49	0.42
1:A:1282:GLN:HA	1:A:1282:GLN:OE1	2.19	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:1297:GLU:O	1:A:1298:VAL:C	2.58	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
2:C:24:ALA:O	2:C:25:ALA:C	2.55	0.42
1:A:1504:GLU:HG3	1:A:1505:VAL:N	2.32	0.42
1:A:1371:LEU:HA	1:A:1375:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ARG:CG	1:A:1273:SER:N	2.81	0.42
1:B:1484:ASN:OD1	2:D:27:M3L:HM22	2.18	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:B:1192:SER:HB2	1:B:1195:ASP:CG	2.40	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:H	1:B:1224:LEU:CD1	2.32	0.41
1:B:1399:VAL:HG11	1:B:1483:TRP:CZ2	2.55	0.41
1:A:1563:TYR:CE1	1:A:1623:ARG:HG3	2.55	0.41
1:A:1190:LEU:HA	1:A:1190:LEU:HD23	1.84	0.41
1:B:1293:GLN:O	1:B:1297:GLU:HG2	2.20	0.41
1:A:1341:LYS:CG	1:A:1345:GLN:OE1	2.68	0.41
1:A:1427:ARG:HG3	1:A:1427:ARG:NH1	2.35	0.41
1:A:1526:LYS:HA	1:A:1526:LYS:HD3	1.96	0.41
1:A:1362:MET:HG3	1:A:1488:LEU:HD23	2.02	0.41
1:A:1413:VAL:HG12	1:A:1414:HIS:N	2.35	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:1519:TRP:CD2	1:A:1540:LEU:HD22	2.56	0.41
1:A:1394:ASN:O	1:A:1496:ALA:HA	2.20	0.41
1:B:1519:TRP:CD2	1:B:1540:LEU:HD22	2.56	0.41
1:B:1422:SER:HA	1:B:1432:TYR:CD1	2.56	0.41
1:B:1167:LYS:HG2	6:B:1831:HOH:O	2.21	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:A:1607:ARG:C	1:A:1609:ARG:N	2.73	0.41
1:B:1536:ILE:O	1:B:1540:LEU:HG	2.21	0.41
1:B:1519:TRP:CE2	1:B:1540:LEU:HD22	2.56	0.41
1:A:1497:LEU:HA	1:A:1497:LEU:HD12	1.85	0.41
1:B:1266:TRP:HB2	1:B:1267:PRO:HD3	2.02	0.41
1:A:1399:VAL:HG11	1:A:1483:TRP:CZ2	2.56	0.41
1:B:1341:LYS:O	1:B:1345:GLN:HG3	2.21	0.40
1:A:1566:ARG:HG3	1:A:1622:TYR:CZ	2.56	0.40
1:A:1359:THR:HG23	1:B:1429:GLY:O	2.20	0.40
1:B:1361:ASN:O	1:B:1362:MET:C	2.59	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:1586:LEU:HD23	1:B:1586:LEU:N	2.35	0.40
1:B:1242:THR:CG2	1:B:1243:VAL:N	2.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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 (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	449/486 (92%)	425 (95%)	23 (5%)	1 (0%)	52 74
1	B	443/486 (91%)	424 (96%)	18 (4%)	1 (0%)	52 74
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%)	52 74

All (2) Ramachandran outliers are listed below:

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

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	404/424 (95%)	371 (92%)	33 (8%)	14 26
1	B	400/424 (94%)	364 (91%)	36 (9%)	12 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	4/4 (100%)	2 (50%)	2 (50%)	0 0
2	D	4/4 (100%)	3 (75%)	1 (25%)	1 1
All	All	812/856 (95%)	740 (91%)	72 (9%)	12 22

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1157	GLU
1	A	1174	GLU
1	A	1175	LYS
1	A	1187	SER
1	A	1191	GLU
1	A	1192	SER
1	A	1200	VAL
1	A	1218	LEU
1	A	1232	LYS
1	A	1242	THR
1	A	1243	VAL
1	A	1253	SER
1	A	1262	THR
1	A	1263	ARG
1	A	1273	SER
1	A	1275	THR
1	A	1287	SER
1	A	1292	LEU
1	A	1300	PHE
1	A	1301	GLN
1	A	1328	PHE
1	A	1341	LYS
1	A	1419	GLU
1	A	1497	LEU
1	A	1504	GLU
1	A	1510	SER
1	A	1523	ARG
1	A	1528	SER
1	A	1560	LYS
1	A	1599	LEU
1	A	1608	ARG
1	A	1609	ARG
1	A	1614	GLN
1	B	1157	GLU

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Mol	Chain	Res	Type
1	B	1175	LYS
1	B	1179	GLU
1	B	1187	SER
1	B	1190	LEU
1	B	1193	LYS
1	B	1214	VAL
1	B	1221	SER
1	B	1238	SER
1	B	1242	THR
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	1300	PHE
1	B	1327	LYS
1	B	1328	PHE
1	B	1339	ARG
1	B	1387	THR
1	B	1390	HIS
1	B	1403	ILE
1	B	1419	GLU
1	B	1497	LEU
1	B	1504	GLU
1	B	1510	SER
1	B	1523	ARG
1	B	1528	SER
1	B	1546	HIS
1	B	1560	LYS
1	B	1586	LEU
1	B	1609	ARG
1	B	1614	GLN
2	C	26	ARG
2	C	32	THR
2	D	26	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1251	GLN
1	A	1256	ASN
1	A	1416	HIS
1	A	1621	GLN
1	B	1251	GLN
1	B	1264	GLN
1	B	1393	ASN
1	B	1473	GLN
1	B	1516	HIS
1	B	1576	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.87	3 (30%)	12,14,16	0.73	0
2	M3L	D	27	2	10,11,12	0.83	0	12,14,16	0.93	1 (8%)

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	-	0/8/10/12	0/0/0/0
2	M3L	D	27	2	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	27	M3L	CB-CA	-3.85	1.50	1.53
2	C	27	M3L	CM2-NZ	-3.05	1.41	1.50
2	C	27	M3L	CE-NZ	-2.36	1.43	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	27	M3L	O-C-CA	-3.05	117.54	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	27	M3L	3	0
2	D	27	M3L	6	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	A	1703	3	3,9,9	0.42	0	3,11,11	0.58	0
5	OGA	B	1703	3	3,9,9	0.63	0	3,11,11	0.71	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	A	1703	3	-	0/3/9/9	0/0/0/0
5	OGA	B	1703	3	-	0/3/9/9	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.

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, 95^{th} 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%)	0.37	34 (7%) 17 19	24, 53, 94, 122	0
1	B	451/486 (92%)	0.31	25 (5%) 29 33	36, 54, 92, 119	0
2	C	10/11 (90%)	0.83	2 (20%) 1 1	58, 81, 109, 109	0
2	D	10/11 (90%)	1.10	1 (10%) 9 10	53, 76, 115, 118	0
All	All	926/994 (93%)	0.35	62 (6%) 21 24	24, 54, 95, 122	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1298	VAL	7.4
1	B	1299	LEU	7.1
1	A	1299	LEU	7.0
1	A	1174	GLU	5.8
1	B	1253	SER	5.0
1	B	1611	ALA	4.5
1	A	1175	LYS	4.5
1	B	1252	PRO	4.3
1	A	1171	ASN	4.3
1	B	1169	LYS	4.0
1	A	1298	VAL	3.9
1	A	1611	ALA	3.8
1	B	1170	ILE	3.8
1	A	1172	THR	3.6
1	A	1173	GLU	3.5
1	B	1606	ALA	3.2
1	B	1610	SER	3.1
1	A	1294	GLU	3.1
1	A	1617	VAL	3.0
1	A	1228	LEU	2.9
1	A	1191	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1575	CYS	2.9
1	A	1180	LYS	2.9
1	B	1612	GLY	2.8
1	A	1598	TYR	2.8
1	A	1597	THR	2.8
1	B	1271	SER	2.8
1	B	1323	HIS	2.7
1	A	1546	HIS	2.7
1	B	1598	TYR	2.7
2	C	28	SER	2.7
2	C	24	ALA	2.7
1	A	1363	LEU	2.6
1	B	1177	PRO	2.6
1	B	1613	LEU	2.5
1	B	1175	LYS	2.5
1	A	1301	GLN	2.4
1	B	1615	GLY	2.4
1	A	1397	CYS	2.3
1	A	1616	VAL	2.3
1	B	1568	LYS	2.3
1	A	1362	MET	2.3
1	B	1254	ASP	2.3
1	A	1615	GLY	2.3
1	A	1485	VAL	2.2
1	A	1398	SER	2.2
1	B	1270	SER	2.2
1	A	1484	ASN	2.2
1	A	1486	GLY	2.2
1	A	1189	TYR	2.2
1	A	1613	LEU	2.2
1	A	1225	ASN	2.2
1	A	1610	SER	2.1
1	A	1356	VAL	2.1
1	B	1290	GLU	2.1
1	B	1324	HIS	2.1
1	B	1176	LEU	2.1
1	B	1614	GLN	2.0
2	D	34	GLY	2.0
1	A	1192	SER	2.0
1	A	1589	THR	2.0
1	A	1399	VAL	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. 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, 95^{th} 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(Å^2)	Q<0.9
2	M3L	D	27	12/13	0.83	0.30	-	48,66,75,78	0
2	M3L	C	27	12/13	0.89	0.27	-	44,62,69,72	0

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, 95^{th} 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(Å^2)	Q<0.9
5	OGA	B	1703	10/10	0.88	0.25	3.20	20,20,20,20	0
5	OGA	A	1703	10/10	0.90	0.21	0.57	20,20,20,20	0
4	ZN	B	1702	1/1	0.96	0.14	-0.78	57,57,57,57	0
4	ZN	A	1702	1/1	0.97	0.09	-2.70	56,56,56,56	0
3	NI	A	1701	1/1	0.95	0.20	-	34,34,34,34	0
3	NI	B	1701	1/1	0.94	0.20	-	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.