



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:04 AM UTC

PDB ID : 4EZ4 / pdb_00004ez4
Title : free KDM6B structure
Authors : Cheng, Z.J.; Patel, D.J.
Deposited on : 2012-05-02
Resolution : 2.99 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

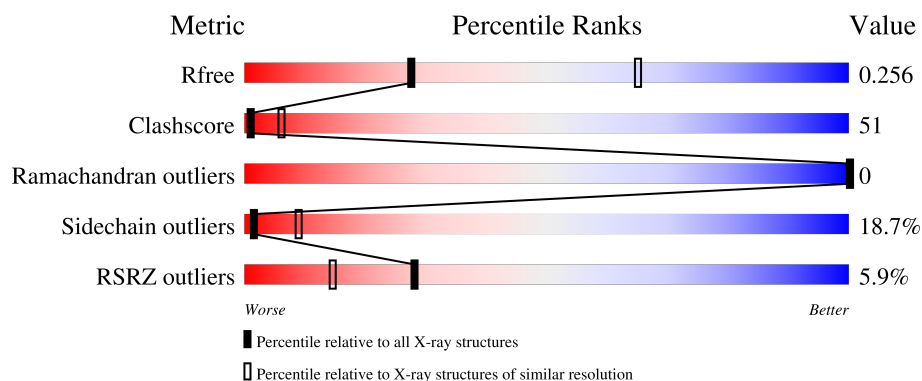
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	5% 37% 44% 12% 8%
1	B	486	6% 40% 41% 11% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7268 atoms, of which 32 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	448	Total	C	H	N	O	S	0	1	0
			3620	2293	16	625	667	19			
1	B	447	Total	C	H	N	O	S	0	1	0
			3612	2290	16	627	660	19			

There are 52 discrepancies between the modelled and reference sequences:

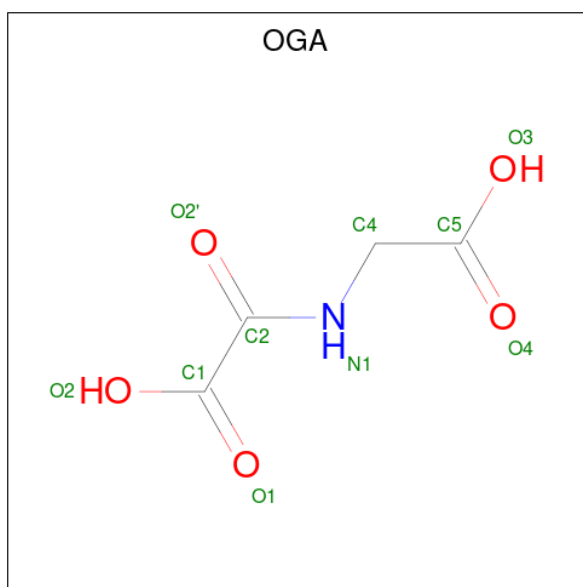
Chain	Residue	Modelled	Actual	Comment	Reference
A	1297	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1298	GLU	-	SEE REMARK 999	UNP Q5NCY0
A	1299	VAL	-	SEE REMARK 999	UNP Q5NCY0
A	1300	LEU	-	SEE REMARK 999	UNP Q5NCY0
A	1301	PHE	-	SEE REMARK 999	UNP Q5NCY0
A	1302	GLN	-	SEE REMARK 999	UNP Q5NCY0
A	1303	GLY	-	SEE REMARK 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	1297	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1298	GLU	-	SEE REMARK 999	UNP Q5NCY0
B	1299	VAL	-	SEE REMARK 999	UNP Q5NCY0
B	1300	LEU	-	SEE REMARK 999	UNP Q5NCY0
B	1301	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 N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



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

- 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		
3	B	1	Total	Ni	0	0
			1	1		

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		

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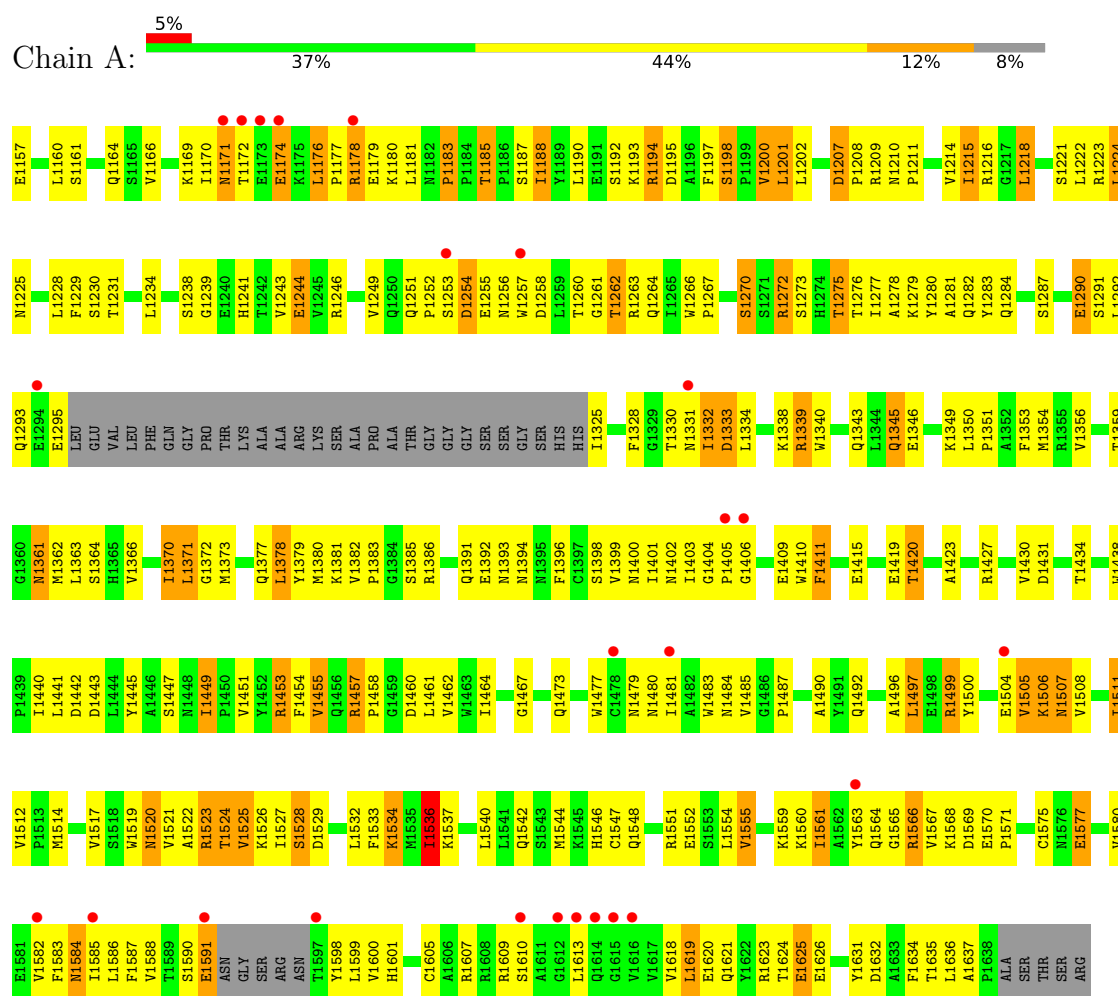
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	7	Total	O	0	0
			7	7		

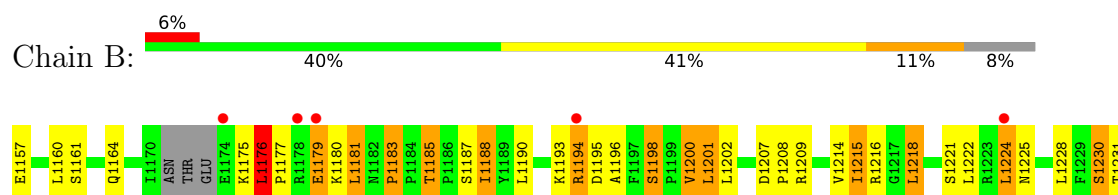
3 Residue-property plots

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



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S1590	S1591	ASN	GLY	SER	ARG	ASN	T1597	S1598	S1599	V1600	H1601	G1602	E1603	G1604	G1605	A1606	G1607	R1608	R1609	S1610	A1611	G1612	L1613	G1614	G1615	V1616	V1617	V1618	L1619	E1620	G1621	V1622	R1623	T1624	E1625	E1626	V1631	A1632	G1633	F1634	T1635	L1636	A1637	P1638	A1639	SER	THR	ARG				
R1523	T1524	R1525	K1526	T1527	S1528	D1529	L1532	F1533	K1534	M1535	R1536	K1537	L1540	L1541	R1542	S1543	M1544	K1545	H1546	G1547	C1548	L1551	R1552	S1553	L1554	V1555	G1558	K1559	L1560	T1561	A1562	F1563	G1564	G1565	R1566	V1567	L1568	D1569	E1570	P1571	C1575	R1576	E1577	C1578	D1579	V1580	E1581	V1582	L1586	F1587	V1588	T1589
L1444	L1445	A1446	S1447	N1448	I1449	P1450	L1452	R1453	F1454	V1455	G1456	R1457	D1460	L1461	V1462	W1463	I1464	G1467	V1472	Q1473	A1474	T1475	G1476	V1477	N1480	I1481	M1484	L1485	G1486	P1487	Q1492	A1496	L1497	F1498	R1499	W1502	N1503	E1504	V1505	K1506	N1507	V1508	K1509	S1510	I1511	V1517	S1518	V1519	V1520			
L1371	G1372	M1373	T1374	N1375	V1376	Q1377	L1378	Y1379	M1380	K1381	P1382	P1383	G1384	R1386	Q1391	E1392	N1393	N1394	N1395	F1396	G1397	S1398	V1399	N1400	I1401	N1402	I1403	P1405	G1406	D1407	C1408	E1409	W1410	F1411	E1415	E1419	T1420	A1423	R1427	G1428	H1429	V1430	D1431	T1434	W1438	P1439	I1440	L1441	D1442			
L1234	PHE	GLN	GLY	PRO	THR	LYS	ALA	ARG	LYS	SER	ALA	ALA	THR	GLY	GLY	GLY	SER	GLY	GLY	H1323	H1324	I1325	I1326	T1263	Q1264	W1266	C1268	E1269	L1334	S1335	D1336	A1337	K1338	R1339	W1340	Q1343	L1344	Q1345	P1351	A1352	F1355	M1354	N1361	M1362	L1363	S1364	H1365	G1367	LEU	GLU	VAL	
S1238	S1239	H1241	V1242	E1244	V1243	V1245	R1246	V1249	Q1250	Q1251	P1252	S1253	D1254	E1255	N1256	S1257	D1258	L1259	T1260	G1261	I1262	T1263	Q1264	W1266	C1268	E1269	L1334	S1335	D1336	A1337	K1338	R1339	W1340	Q1343	L1344	Q1345	P1351	A1352	F1355	M1354	N1361	M1362	L1363	S1364	H1365	G1367	LEU	GLU	VAL			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.66Å 123.71Å 82.04Å 90.00° 109.62° 90.00°	Depositor
Resolution (Å)	49.73 – 2.99 49.73 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.73-2.99) 95.6 (49.73-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.190 , 0.250 0.211 , 0.256	Depositor DCC
R_{free} test set	1079 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 25.76 % 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 2.9848e-03. 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: NI, ZN, 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	0.64	2/3700 (0.1%)	1.06	14/5035 (0.3%)
1	B	0.65	2/3693 (0.1%)	1.09	15/5024 (0.3%)
All	All	0.65	4/7393 (0.1%)	1.07	29/10059 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1361	ASN	CG-ND2	-6.08	1.20	1.33
1	B	1361	ASN	CG-OD1	-5.60	1.12	1.23
1	A	1361	ASN	CG-ND2	-5.44	1.21	1.33
1	A	1361	ASN	CG-OD1	-5.16	1.13	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1183	PRO	O-C-N	7.96	124.89	121.15
1	A	1536	ILE	N-CA-C	-7.68	102.96	110.72
1	B	1176	LEU	CA-C-N	7.20	127.12	120.21
1	B	1176	LEU	C-N-CA	7.20	127.12	120.21
1	A	1198	SER	CA-C-N	7.05	126.67	119.19
1	A	1198	SER	C-N-CA	7.05	126.67	119.19
1	B	1198	SER	CA-C-N	7.00	126.61	119.19
1	B	1198	SER	C-N-CA	7.00	126.61	119.19
1	B	1183	PRO	CA-C-N	6.76	126.52	119.76
1	B	1183	PRO	C-N-CA	6.76	126.52	119.76
1	A	1277	ILE	CB-CA-C	-6.55	103.46	112.04
1	A	1406	GLY	N-CA-C	6.53	119.00	111.36
1	A	1183	PRO	CA-C-N	6.36	126.12	119.76
1	A	1183	PRO	C-N-CA	6.36	126.12	119.76
1	B	1230	SER	N-CA-C	-6.27	102.70	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1486	GLY	CA-C-N	-5.75	114.83	120.98
1	B	1486	GLY	C-N-CA	-5.75	114.83	120.98
1	B	1536	ILE	N-CA-C	-5.70	104.97	110.72
1	A	1183	PRO	O-C-N	5.52	123.74	121.15
1	B	1533	PHE	CA-C-N	5.39	127.77	120.38
1	B	1533	PHE	C-N-CA	5.39	127.77	120.38
1	A	1512	VAL	N-CA-C	5.25	113.61	107.89
1	B	1507	ASN	N-CA-C	-5.09	105.91	113.40
1	A	1350	LEU	CA-C-N	5.08	125.36	119.92
1	A	1350	LEU	C-N-CA	5.08	125.36	119.92
1	A	1449	ILE	N-CA-C	5.08	113.04	107.60
1	B	1253	SER	N-CA-C	5.08	117.47	111.33
1	A	1207	ASP	CA-C-N	5.03	124.69	119.56
1	A	1207	ASP	C-N-CA	5.03	124.69	119.56

There are no chirality outliers.

There are no planarity outliers.

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	3604	16	3524	373	0
1	B	3596	16	3517	381	0
2	A	10	0	3	2	0
2	B	10	0	3	1	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	5	0	0	0	0
5	B	7	0	0	0	0
All	All	7236	32	7047	730	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 51.

All (730) 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:A:1193:LYS:CE	1:B:1578:CYS:HA	1.53	1.38
1:B:1568:LYS:HE3	1:B:1568:LYS:CA	1.41	1.37
1:A:1215:ILE:HD12	1:A:1215:ILE:O	1.17	1.32
1:B:1215:ILE:O	1:B:1215:ILE:HD12	1.21	1.27
1:A:1339:ARG:HH11	1:A:1339:ARG:CB	1.46	1.26
1:B:1568:LYS:HA	1:B:1568:LYS:CE	1.58	1.25
1:A:1339:ARG:HB2	1:A:1339:ARG:NH1	1.49	1.24
1:B:1563:TYR:CE1	1:B:1623:ARG:HG2	1.75	1.21
1:B:1568:LYS:CE	1:B:1569:ASP:H	1.57	1.16
1:B:1566:ARG:NH1	1:B:1570:GLU:HG2	1.60	1.15
1:B:1339:ARG:HG2	1:B:1339:ARG:HH21	1.08	1.13
1:A:1332:ILE:HD12	1:A:1378:LEU:HD23	1.19	1.12
1:A:1371:LEU:H	1:A:1371:LEU:HD12	1.09	1.12
1:B:1371:LEU:HD12	1:B:1371:LEU:H	1.14	1.11
1:A:1177:PRO:HD2	1:A:1180:LYS:HG2	1.33	1.08
1:B:1568:LYS:HE2	1:B:1569:ASP:H	1.00	1.07
1:B:1332:ILE:HD12	1:B:1378:LEU:HD23	1.37	1.06
1:A:1193:LYS:HE3	1:B:1578:CYS:HA	1.12	1.06
1:B:1215:ILE:CD1	1:B:1218:LEU:HB3	1.86	1.05
1:B:1536:ILE:HD12	1:B:1536:ILE:C	1.82	1.04
1:A:1582:VAL:HG12	1:A:1586:LEU:CD2	1.87	1.04
1:A:1371:LEU:HD12	1:A:1371:LEU:N	1.67	1.03
1:B:1563:TYR:HE1	1:B:1623:ARG:HG2	1.04	1.03
1:B:1564:GLN:HE21	1:B:1565:GLY:H	1.04	1.03
1:A:1215:ILE:O	1:A:1215:ILE:CD1	2.08	1.02
1:A:1215:ILE:CD1	1:A:1218:LEU:HB3	1.89	1.02
1:A:1536:ILE:C	1:A:1536:ILE:HD12	1.85	1.01
1:B:1339:ARG:HH21	1:B:1339:ARG:CG	1.73	1.01
1:B:1527:ILE:HD13	1:B:1533:PHE:HB2	1.43	1.01
1:B:1399:VAL:HG13	1:B:1461:LEU:HD11	1.42	1.01
1:B:1371:LEU:HD12	1:B:1371:LEU:N	1.71	1.00
1:A:1272:ARG:CZ	1:A:1272:ARG:HB3	1.88	1.00
1:A:1399:VAL:HG13	1:A:1461:LEU:HD11	1.42	0.99
1:B:1568:LYS:CE	1:B:1569:ASP:N	2.25	0.99
1:A:1566:ARG:HH11	1:A:1566:ARG:HG2	1.25	0.98
1:B:1215:ILE:O	1:B:1215:ILE:CD1	2.12	0.98
1:B:1272:ARG:CZ	1:B:1272:ARG:HB3	1.90	0.97
1:B:1568:LYS:HE3	1:B:1568:LYS:C	1.90	0.97
1:B:1568:LYS:CA	1:B:1568:LYS:CE	2.30	0.97
1:A:1215:ILE:HD12	1:A:1215:ILE:C	1.90	0.96
1:B:1164:GLN:NE2	1:B:1534:LYS:HG3	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1272:ARG:HB3	1:B:1272:ARG:NH1	1.80	0.96
1:B:1215:ILE:HD11	1:B:1218:LEU:HB3	1.47	0.96
1:B:1568:LYS:HE2	1:B:1569:ASP:N	1.80	0.95
1:A:1272:ARG:HB3	1:A:1272:ARG:NH1	1.81	0.95
1:A:1527:ILE:HD13	1:A:1533:PHE:HB2	1.45	0.94
1:A:1193:LYS:NZ	1:B:1578:CYS:HA	1.82	0.93
1:A:1332:ILE:CD1	1:A:1378:LEU:HD23	1.99	0.93
1:B:1177:PRO:HD2	1:B:1180:LYS:HG2	1.51	0.93
1:A:1160:LEU:HG	1:A:1497:LEU:HD23	1.51	0.93
1:A:1371:LEU:H	1:A:1371:LEU:CD1	1.82	0.92
1:B:1215:ILE:HD12	1:B:1215:ILE:C	1.94	0.92
1:A:1339:ARG:HH11	1:A:1339:ARG:HB2	0.76	0.92
1:A:1527:ILE:HD12	1:A:1636:LEU:HD12	1.51	0.91
1:B:1566:ARG:HH12	1:B:1570:GLU:HG2	1.29	0.89
1:B:1371:LEU:H	1:B:1371:LEU:CD1	1.85	0.89
1:B:1164:GLN:HE22	1:B:1534:LYS:HG3	1.37	0.87
1:B:1160:LEU:HG	1:B:1497:LEU:HD23	1.53	0.87
1:A:1177:PRO:CD	1:A:1180:LYS:HG2	2.05	0.87
1:A:1171:ASN:H	1:A:1171:ASN:ND2	1.71	0.87
1:A:1276:THR:OG1	1:A:1278:ALA:HB3	1.75	0.87
1:B:1177:PRO:CD	1:B:1180:LYS:HG2	2.05	0.87
1:A:1215:ILE:HD13	1:A:1218:LEU:HB3	1.56	0.87
1:A:1536:ILE:HD11	1:A:1634:PHE:CE2	2.10	0.86
1:A:1566:ARG:HH11	1:A:1566:ARG:CG	1.89	0.86
1:B:1563:TYR:CE1	1:B:1623:ARG:CG	2.59	0.86
1:B:1177:PRO:CG	1:B:1180:LYS:HG2	2.04	0.86
1:B:1339:ARG:HG2	1:B:1339:ARG:NH2	1.71	0.85
1:A:1582:VAL:HG12	1:A:1586:LEU:HD23	1.58	0.85
1:A:1528:SER:HA	1:A:1637:ALA:O	1.77	0.85
1:B:1201:LEU:HD12	1:B:1201:LEU:C	2.01	0.85
1:B:1506:LYS:O	1:B:1507:ASN:HB2	1.75	0.85
1:B:1276:THR:OG1	1:B:1279:LYS:HG3	1.77	0.84
1:B:1566:ARG:NH1	1:B:1570:GLU:CG	2.40	0.84
1:A:1266:TRP:CD1	1:A:1440:ILE:HD12	2.12	0.84
1:A:1170:ILE:HG22	1:A:1170:ILE:O	1.75	0.84
1:B:1597:THR:O	1:B:1598:TYR:CD2	2.30	0.84
1:A:1193:LYS:HE3	1:B:1578:CYS:CA	2.02	0.84
1:A:1160:LEU:CG	1:A:1497:LEU:HD23	2.07	0.83
1:A:1215:ILE:HD11	1:A:1218:LEU:HB3	1.58	0.83
1:A:1447:SER:HB2	1:A:1449:ILE:HG13	1.58	0.83
1:A:1555:VAL:HG23	1:A:1561:ILE:HD11	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1563:TYR:CD1	1:B:1623:ARG:NE	2.46	0.83
1:B:1607:ARG:NH2	1:B:1613:LEU:CD1	2.42	0.83
1:A:1160:LEU:CD2	1:A:1497:LEU:HD23	2.09	0.82
1:A:1506:LYS:O	1:A:1507:ASN:HB2	1.78	0.82
1:B:1160:LEU:CD2	1:B:1497:LEU:HD23	2.09	0.82
1:B:1333:ASP:C	1:B:1334:LEU:HD23	2.04	0.82
1:B:1536:ILE:HD11	1:B:1634:PHE:CE2	2.15	0.82
1:B:1272:ARG:NH1	1:B:1272:ARG:CB	2.42	0.82
1:B:1536:ILE:HD12	1:B:1536:ILE:O	1.79	0.82
1:B:1160:LEU:CG	1:B:1497:LEU:HD23	2.09	0.82
1:A:1215:ILE:CD1	1:A:1215:ILE:C	2.50	0.81
1:B:1215:ILE:HD13	1:B:1218:LEU:HB3	1.62	0.81
1:B:1215:ILE:CD1	1:B:1218:LEU:CB	2.58	0.81
1:B:1568:LYS:HE3	1:B:1569:ASP:N	1.89	0.81
1:B:1607:ARG:NH2	1:B:1613:LEU:HD11	1.96	0.81
1:A:1333:ASP:C	1:A:1334:LEU:HD23	2.06	0.80
1:B:1555:VAL:HG23	1:B:1561:ILE:HD11	1.62	0.80
1:A:1193:LYS:CE	1:B:1578:CYS:CA	2.49	0.80
1:A:1527:ILE:HD11	1:A:1533:PHE:CD1	2.17	0.80
1:A:1582:VAL:CG1	1:A:1586:LEU:CD2	2.60	0.80
1:A:1177:PRO:HD2	1:A:1180:LYS:CG	2.11	0.80
1:A:1193:LYS:NZ	1:B:1578:CYS:CA	2.45	0.80
1:A:1215:ILE:HD13	1:A:1218:LEU:CB	2.12	0.80
1:B:1215:ILE:CD1	1:B:1215:ILE:C	2.53	0.80
1:B:1563:TYR:CE2	1:B:1564:GLN:O	2.34	0.80
1:A:1201:LEU:C	1:A:1201:LEU:HD12	2.07	0.79
1:A:1164:GLN:NE2	1:A:1534:LYS:HD2	1.97	0.79
1:A:1398:SER:HB3	1:A:1464:ILE:HD13	1.63	0.79
1:B:1527:ILE:O	1:B:1527:ILE:HD12	1.82	0.79
1:B:1527:ILE:HD11	1:B:1533:PHE:CD1	2.18	0.79
1:B:1177:PRO:HG2	1:B:1180:LYS:HG2	1.64	0.78
1:B:1398:SER:HB3	1:B:1464:ILE:HD13	1.65	0.78
1:B:1215:ILE:HD13	1:B:1218:LEU:CB	2.14	0.78
1:B:1638:PRO:O	1:B:1639:ALA:CB	2.31	0.78
1:B:1381:LYS:HE3	1:B:1480:ASN:OD1	1.84	0.78
1:B:1266:TRP:CD1	1:B:1440:ILE:HD12	2.20	0.77
1:A:1215:ILE:HG13	1:A:1461:LEU:HB3	1.66	0.77
1:A:1536:ILE:HD12	1:A:1536:ILE:O	1.83	0.77
1:A:1351:PRO:HG2	1:A:1354:MET:HE3	1.67	0.77
1:A:1272:ARG:NH1	1:A:1272:ARG:CB	2.48	0.76
1:B:1215:ILE:HG13	1:B:1461:LEU:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1564:GLN:HE21	1:B:1565:GLY:N	1.82	0.76
1:B:1568:LYS:HE3	1:B:1568:LYS:HA	0.77	0.76
1:A:1582:VAL:HG12	1:A:1586:LEU:HD22	1.68	0.76
1:A:1164:GLN:NE2	1:A:1534:LYS:HG3	2.00	0.76
1:A:1215:ILE:CD1	1:A:1218:LEU:CB	2.63	0.76
1:A:1334:LEU:HD23	1:A:1334:LEU:N	2.01	0.76
1:B:1187:SER:O	1:B:1188:ILE:HD13	1.86	0.75
1:A:1174:GLU:O	1:A:1176:LEU:HD12	1.86	0.75
1:B:1447:SER:HB2	1:B:1449:ILE:HG13	1.66	0.75
1:A:1582:VAL:CG1	1:A:1586:LEU:HD22	2.16	0.75
1:A:1176:LEU:HD12	1:A:1176:LEU:N	2.00	0.75
1:B:1243:VAL:HG11	1:B:1277:ILE:HG12	1.67	0.75
1:B:1370:ILE:HG21	1:B:1511:ILE:HG23	1.68	0.75
1:A:1381:LYS:HE3	1:A:1480:ASN:OD1	1.87	0.74
1:B:1334:LEU:HD23	1:B:1334:LEU:N	2.00	0.74
1:A:1519:TRP:CE2	1:A:1540:LEU:HD22	2.23	0.73
1:A:1332:ILE:HD12	1:A:1378:LEU:CD2	2.10	0.73
1:B:1243:VAL:CG1	1:B:1277:ILE:HG12	2.18	0.73
1:A:1370:ILE:HG21	1:A:1511:ILE:HG23	1.71	0.73
1:B:1331:ASN:HA	1:B:1377:GLN:NE2	2.04	0.73
1:B:1267:PRO:HG3	1:B:1430:VAL:CG2	2.19	0.72
1:B:1563:TYR:C	1:B:1563:TYR:CD2	2.67	0.72
1:A:1527:ILE:CD1	1:A:1533:PHE:CD1	2.72	0.72
1:B:1336:ASP:OD2	1:B:1339:ARG:HG3	1.89	0.72
1:B:1533:PHE:CE2	1:B:1636:LEU:CD2	2.72	0.72
1:B:1582:VAL:HG11	1:B:1586:LEU:HB3	1.70	0.72
1:B:1394:ASN:HA	1:B:1499:ARG:HG2	1.70	0.72
1:A:1255:GLU:HB2	1:A:1257:TRP:NE1	2.05	0.71
1:B:1638:PRO:O	1:B:1639:ALA:HB2	1.89	0.71
1:A:1399:VAL:CG1	1:A:1461:LEU:HD11	2.20	0.71
1:B:1398:SER:HB3	1:B:1464:ILE:CD1	2.20	0.71
1:A:1171:ASN:ND2	1:A:1171:ASN:N	2.34	0.71
1:A:1623:ARG:HB2	1:A:1626:GLU:HG3	1.73	0.71
1:B:1607:ARG:CZ	1:B:1613:LEU:HD11	2.21	0.71
1:B:1527:ILE:CD1	1:B:1533:PHE:CD1	2.74	0.71
1:A:1194:ARG:HG3	1:A:1195:ASP:H	1.56	0.71
1:B:1399:VAL:CG1	1:B:1461:LEU:HD11	2.19	0.71
1:B:1164:GLN:NE2	1:B:1534:LYS:CG	2.53	0.71
1:B:1214:VAL:HG22	1:B:1454:PHE:CE1	2.26	0.71
1:B:1328:PHE:HE1	1:B:1381:LYS:HG2	1.55	0.71
1:B:1563:TYR:CD2	1:B:1564:GLN:O	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1176:LEU:HD12	1:B:1176:LEU:N	2.05	0.70
1:A:1193:LYS:HZ1	1:B:1578:CYS:C	1.98	0.70
1:A:1284:GLN:HE22	1:A:1380:MET:HB3	1.56	0.70
1:B:1332:ILE:CD1	1:B:1378:LEU:HD23	2.18	0.70
1:A:1193:LYS:HZ1	1:B:1578:CYS:CA	2.05	0.70
1:A:1257:TRP:CD2	1:A:1264:GLN:HG3	2.26	0.70
1:A:1187:SER:O	1:A:1188:ILE:HD13	1.91	0.69
1:A:1239:GLY:O	1:A:1278:ALA:HB2	1.92	0.69
1:A:1257:TRP:CE3	1:A:1264:GLN:HG3	2.27	0.69
1:B:1527:ILE:HD13	1:B:1533:PHE:CB	2.21	0.69
1:A:1328:PHE:HE1	1:A:1381:LYS:HG2	1.58	0.69
1:A:1398:SER:HB3	1:A:1464:ILE:CD1	2.22	0.69
1:B:1177:PRO:HD2	1:B:1180:LYS:CG	2.22	0.69
1:A:1276:THR:HG23	1:A:1279:LYS:HE3	1.75	0.69
1:A:1525:VAL:HG13	1:A:1526:LYS:O	1.92	0.69
1:B:1284:GLN:HE22	1:B:1380:MET:HB3	1.57	0.69
1:B:1597:THR:HG22	1:B:1598:TYR:HD2	1.57	0.69
1:A:1214:VAL:HG22	1:A:1454:PHE:CE1	2.28	0.69
1:B:1564:GLN:NE2	1:B:1565:GLY:H	1.85	0.69
1:B:1372:GLY:HA2	1:B:1377:GLN:HG2	1.75	0.68
1:A:1192:SER:HB3	1:B:1577:GLU:HB3	1.74	0.68
1:B:1623:ARG:HB2	1:B:1626:GLU:HG3	1.74	0.68
1:B:1272:ARG:CG	1:B:1272:ARG:HH11	2.06	0.68
1:B:1351:PRO:HG2	1:B:1354:MET:HE3	1.76	0.68
1:A:1267:PRO:HG3	1:A:1430:VAL:CG2	2.24	0.68
1:B:1362:MET:HE3	1:B:1487:PRO:O	1.94	0.68
1:A:1423:ALA:HB1	1:A:1427:ARG:HH21	1.57	0.68
1:A:1185:THR:HG21	1:A:1454:PHE:CD2	2.29	0.68
1:B:1423:ALA:HB1	1:B:1427:ARG:HH21	1.59	0.68
1:B:1525:VAL:HG13	1:B:1526:LYS:O	1.95	0.67
1:A:1372:GLY:HA2	1:A:1377:GLN:HG2	1.76	0.67
1:B:1175:LYS:HG3	1:B:1176:LEU:N	2.08	0.67
1:B:1272:ARG:NH1	1:B:1272:ARG:N	2.41	0.67
1:A:1394:ASN:HA	1:A:1499:ARG:HG2	1.77	0.67
1:A:1537:LYS:HE3	1:A:1634:PHE:O	1.94	0.67
1:A:1238:SER:OG	1:A:1241:HIS:HB2	1.95	0.67
1:B:1406:GLY:HA3	1:B:1476:GLY:HA3	1.76	0.67
1:A:1536:ILE:C	1:A:1536:ILE:CD1	2.58	0.67
1:B:1272:ARG:NH1	1:B:1272:ARG:H	1.91	0.67
1:B:1194:ARG:CB	1:B:1194:ARG:HH21	2.07	0.67
1:A:1339:ARG:CB	1:A:1339:ARG:NH1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:GLU:OE1	1:A:1349:LYS:NZ	2.26	0.66
1:B:1386:ARG:HD3	1:B:1438:TRP:CE3	2.30	0.66
1:A:1164:GLN:NE2	1:A:1534:LYS:CG	2.57	0.66
1:B:1253:SER:HA	1:B:1473:GLN:NE2	2.11	0.66
1:A:1188:ILE:O	1:A:1216:ARG:N	2.22	0.66
1:A:1171:ASN:N	1:A:1171:ASN:HD22	1.93	0.66
1:B:1188:ILE:O	1:B:1216:ARG:N	2.22	0.66
1:A:1349:LYS:HE2	1:B:1505:VAL:O	1.96	0.65
1:B:1563:TYR:HD2	1:B:1563:TYR:O	1.78	0.65
1:B:1519:TRP:CD2	1:B:1540:LEU:HD22	2.31	0.65
1:A:1176:LEU:N	1:A:1176:LEU:CD1	2.59	0.65
1:B:1272:ARG:CB	1:B:1272:ARG:HH11	2.09	0.65
1:A:1363:LEU:HD21	1:A:1396:PHE:CD1	2.31	0.65
1:A:1527:ILE:HD12	1:A:1527:ILE:O	1.96	0.65
1:A:1519:TRP:CD2	1:A:1540:LEU:HD22	2.31	0.65
1:A:1253:SER:HA	1:A:1473:GLN:NE2	2.11	0.65
1:B:1536:ILE:C	1:B:1536:ILE:CD1	2.55	0.65
1:B:1607:ARG:NH2	1:B:1613:LEU:HD12	2.11	0.65
1:A:1255:GLU:HB2	1:A:1257:TRP:HE1	1.61	0.65
1:A:1577:GLU:HG3	1:A:1605:CYS:HB3	1.79	0.64
1:A:1585:ILE:HA	1:A:1619:LEU:O	1.96	0.64
1:A:1386:ARG:CG	1:A:1438:TRP:CZ3	2.80	0.64
1:A:1527:ILE:HD13	1:A:1533:PHE:CB	2.24	0.64
1:A:1527:ILE:CD1	1:A:1636:LEU:HD12	2.27	0.64
1:A:1536:ILE:CD1	1:A:1634:PHE:CE2	2.80	0.64
1:B:1536:ILE:CD1	1:B:1540:LEU:HD12	2.26	0.64
1:A:1164:GLN:HE22	1:A:1534:LYS:HD2	1.62	0.64
1:A:1386:ARG:HD3	1:A:1438:TRP:CE3	2.33	0.64
1:B:1563:TYR:HE1	1:B:1623:ARG:CG	1.94	0.64
1:B:1533:PHE:CE2	1:B:1636:LEU:HD21	2.33	0.63
1:A:1258:ASP:OD1	1:A:1261:GLY:N	2.32	0.63
1:A:1536:ILE:HG12	1:A:1634:PHE:CZ	2.33	0.63
1:A:1607:ARG:CZ	1:A:1613:LEU:HD11	2.27	0.63
1:A:1359:THR:HG23	1:B:1429:GLY:O	1.98	0.63
1:A:1536:ILE:CG1	1:A:1634:PHE:CE2	2.80	0.63
1:B:1544:MET:HE1	1:B:1631:TYR:CG	2.32	0.63
1:A:1215:ILE:CG1	1:A:1461:LEU:HB3	2.28	0.63
1:B:1185:THR:HG21	1:B:1454:PHE:CD2	2.33	0.63
1:B:1536:ILE:HD11	1:B:1540:LEU:HD12	1.81	0.63
1:A:1200:VAL:CG1	1:A:1201:LEU:N	2.62	0.63
1:B:1598:TYR:O	1:B:1599:LEU:HD13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1194:ARG:HH21	1:B:1194:ARG:HB2	1.64	0.63
1:B:1331:ASN:HB3	1:B:1377:GLN:HE22	1.64	0.63
1:A:1582:VAL:CG1	1:A:1586:LEU:HD23	2.28	0.63
1:B:1195:ASP:O	1:B:1198:SER:HB3	1.98	0.62
1:B:1272:ARG:HH11	1:B:1272:ARG:H	1.45	0.62
1:A:1544:MET:HE1	1:A:1631:TYR:CG	2.34	0.62
1:B:1252:PRO:HD2	1:B:1255:GLU:HG3	1.81	0.62
1:B:1536:ILE:CG1	1:B:1634:PHE:CE2	2.81	0.62
1:A:1362:MET:HE3	1:A:1487:PRO:O	2.00	0.62
1:B:1519:TRP:CE2	1:B:1540:LEU:HD22	2.34	0.62
1:A:1590:SER:O	1:A:1591:GLU:O	2.17	0.62
1:B:1563:TYR:CD1	1:B:1623:ARG:HG2	2.32	0.62
1:A:1164:GLN:HE22	1:A:1534:LYS:HG3	1.63	0.62
1:B:1331:ASN:HD22	1:B:1377:GLN:HE21	1.47	0.62
1:B:1176:LEU:HB3	1:B:1177:PRO:HD2	1.80	0.62
1:A:1276:THR:OG1	1:A:1279:LYS:HG3	1.99	0.62
1:A:1527:ILE:HD12	1:A:1636:LEU:CD1	2.26	0.62
1:A:1164:GLN:NE2	1:A:1534:LYS:CD	2.63	0.62
1:B:1533:PHE:CD2	1:B:1636:LEU:HD21	2.35	0.61
1:B:1328:PHE:CE1	1:B:1381:LYS:HG2	2.35	0.61
1:A:1363:LEU:HD21	1:A:1396:PHE:CE1	2.34	0.61
1:A:1536:ILE:CD1	1:A:1540:LEU:HD12	2.30	0.61
1:A:1176:LEU:CD1	1:A:1176:LEU:H	2.14	0.61
1:A:1254:ASP:OD1	1:A:1254:ASP:N	2.23	0.61
1:A:1568:LYS:HG2	1:A:1569:ASP:OD2	2.00	0.61
1:B:1386:ARG:CG	1:B:1438:TRP:CZ3	2.83	0.61
1:A:1588:VAL:HG21	1:A:1619:LEU:HD11	1.82	0.61
1:A:1280:TYR:HE2	1:A:1284:GLN:HE21	1.48	0.61
1:B:1253:SER:HB2	1:B:1411:PHE:HZ	1.66	0.61
1:A:1194:ARG:HG3	1:A:1195:ASP:N	2.13	0.60
1:B:1238:SER:OG	1:B:1241:HIS:HB2	2.00	0.60
1:A:1214:VAL:HG21	1:A:1454:PHE:CD1	2.36	0.60
1:A:1272:ARG:NH1	1:A:1272:ARG:N	2.50	0.60
1:B:1243:VAL:CG1	1:B:1277:ILE:CG1	2.79	0.60
1:B:1506:LYS:O	1:B:1507:ASN:CB	2.49	0.60
1:A:1252:PRO:HD2	1:A:1255:GLU:HG3	1.81	0.60
1:A:1272:ARG:H	1:A:1272:ARG:HH11	1.50	0.60
1:B:1386:ARG:HG3	1:B:1438:TRP:CZ3	2.36	0.60
1:B:1588:VAL:HG21	1:B:1619:LEU:HD11	1.84	0.60
1:B:1202:LEU:HD13	1:B:1353:PHE:CG	2.37	0.60
1:B:1336:ASP:OD2	1:B:1339:ARG:CG	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:GLU:OE2	1:B:1453:ARG:NH2	2.29	0.60
1:B:1536:ILE:HG12	1:B:1634:PHE:CZ	2.36	0.60
1:B:1588:VAL:HA	1:B:1599:LEU:O	2.02	0.60
1:B:1175:LYS:HG3	1:B:1176:LEU:H	1.66	0.60
1:B:1201:LEU:HD11	1:B:1353:PHE:CZ	2.36	0.60
1:A:1201:LEU:HD11	1:A:1353:PHE:CZ	2.36	0.59
1:A:1588:VAL:HA	1:A:1599:LEU:O	2.02	0.59
1:B:1254:ASP:OD1	1:B:1254:ASP:N	2.29	0.59
1:B:1258:ASP:OD1	1:B:1261:GLY:N	2.35	0.59
1:A:1381:LYS:NZ	2:A:1701:OGA:O3	2.32	0.59
1:A:1555:VAL:CG2	1:A:1561:ILE:HD11	2.31	0.59
1:B:1200:VAL:CG1	1:B:1201:LEU:N	2.64	0.59
1:B:1251:GLN:OE1	1:B:1256:ASN:HA	2.02	0.59
1:B:1160:LEU:HD21	1:B:1497:LEU:HD23	1.85	0.59
1:B:1218:LEU:O	1:B:1221:SER:HB3	2.02	0.59
1:A:1253:SER:HB2	1:A:1411:PHE:HZ	1.67	0.59
1:B:1215:ILE:CG1	1:B:1461:LEU:HB3	2.32	0.59
1:B:1536:ILE:CD1	1:B:1540:LEU:CD1	2.81	0.59
1:B:1255:GLU:HB2	1:B:1257:TRP:NE1	2.18	0.59
1:B:1536:ILE:CD1	1:B:1634:PHE:CE2	2.84	0.59
1:A:1195:ASP:O	1:A:1198:SER:HB3	2.03	0.59
1:A:1527:ILE:CD1	1:A:1636:LEU:CD1	2.81	0.59
1:B:1363:LEU:HD21	1:B:1396:PHE:CD1	2.38	0.59
1:A:1386:ARG:HG3	1:A:1438:TRP:CZ3	2.37	0.58
1:A:1177:PRO:CG	1:A:1180:LYS:HG2	2.32	0.58
1:B:1597:THR:HG22	1:B:1598:TYR:CD2	2.36	0.58
1:A:1536:ILE:HD11	1:A:1540:LEU:HD12	1.86	0.58
1:B:1214:VAL:HG21	1:B:1454:PHE:CD1	2.38	0.58
1:B:1334:LEU:HA	1:B:1340:TRP:CD1	2.39	0.58
1:B:1201:LEU:HD11	1:B:1353:PHE:HZ	1.67	0.58
1:B:1230:SER:O	1:B:1234:LEU:HG	2.04	0.58
1:B:1331:ASN:HD22	1:B:1377:GLN:NE2	2.01	0.58
1:A:1334:LEU:HA	1:A:1340:TRP:CD1	2.38	0.58
1:B:1555:VAL:CG2	1:B:1561:ILE:HD11	2.32	0.58
1:A:1485:VAL:O	1:A:1487:PRO:HD3	2.04	0.58
1:A:1160:LEU:HD21	1:A:1497:LEU:HD23	1.83	0.58
1:B:1280:TYR:HE2	1:B:1284:GLN:HE21	1.52	0.57
1:B:1267:PRO:HG3	1:B:1430:VAL:HG21	1.85	0.57
1:A:1201:LEU:HD11	1:A:1353:PHE:HZ	1.69	0.57
1:A:1565:GLY:O	1:A:1566:ARG:CG	2.52	0.57
1:B:1588:VAL:CG1	1:B:1598:TYR:HD1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:ILE:CG1	1:A:1634:PHE:CZ	2.88	0.57
1:A:1193:LYS:HZ3	1:B:1578:CYS:HB2	1.70	0.57
1:A:1272:ARG:CB	1:A:1272:ARG:HH11	2.16	0.57
1:B:1331:ASN:CB	1:B:1377:GLN:HE22	2.18	0.57
1:B:1394:ASN:O	1:B:1496:ALA:HA	2.04	0.57
1:A:1566:ARG:CG	1:A:1566:ARG:NH1	2.57	0.57
1:B:1536:ILE:CG1	1:B:1634:PHE:CZ	2.87	0.57
1:A:1566:ARG:HG2	1:A:1566:ARG:NH1	2.06	0.57
1:A:1455:VAL:HG12	1:A:1457:ARG:HD2	1.87	0.57
1:B:1492:GLN:HE21	1:B:1492:GLN:C	2.11	0.57
1:A:1394:ASN:O	1:A:1496:ALA:HA	2.05	0.56
1:B:1339:ARG:HH21	1:B:1339:ARG:CB	2.17	0.56
1:B:1363:LEU:HD21	1:B:1396:PHE:CE1	2.38	0.56
1:A:1176:LEU:HB3	1:A:1180:LYS:CB	2.36	0.56
1:A:1328:PHE:CE1	1:A:1381:LYS:HG2	2.40	0.56
1:A:1231:THR:OG1	1:A:1380:MET:CE	2.53	0.56
1:A:1340:TRP:O	1:A:1343:GLN:HB2	2.06	0.56
1:B:1597:THR:O	1:B:1598:TYR:CG	2.58	0.56
1:A:1215:ILE:CD1	1:A:1461:LEU:H	2.18	0.56
1:B:1373:MET:SD	1:B:1511:ILE:CG2	2.94	0.56
1:B:1577:GLU:HG3	1:B:1605:CYS:HB3	1.86	0.56
1:B:1588:VAL:HG12	1:B:1598:TYR:HD1	1.69	0.56
1:A:1231:THR:CG2	1:A:1281:ALA:HB1	2.35	0.56
1:A:1280:TYR:C	1:A:1280:TYR:CD2	2.84	0.56
1:A:1346:GLU:OE1	1:A:1349:LYS:HE3	2.05	0.56
1:B:1527:ILE:CD1	1:B:1533:PHE:HD1	2.19	0.56
1:B:1598:TYR:O	1:B:1599:LEU:CD1	2.53	0.56
1:A:1253:SER:CA	1:A:1473:GLN:NE2	2.69	0.56
1:A:1257:TRP:CZ2	1:A:1264:GLN:CD	2.84	0.56
1:A:1366:VAL:HG21	1:A:1370:ILE:HD11	1.87	0.56
1:A:1559:LYS:HE3	1:A:1613:LEU:HB2	1.88	0.56
1:A:1214:VAL:CG2	1:A:1454:PHE:CD1	2.89	0.56
1:A:1246:ARG:HD2	1:A:1270:SER:OG	2.06	0.56
1:B:1533:PHE:CE2	1:B:1636:LEU:HD22	2.41	0.56
1:B:1533:PHE:CZ	1:B:1636:LEU:HD22	2.41	0.56
1:B:1567:VAL:HG23	1:B:1568:LYS:N	2.21	0.56
1:A:1536:ILE:CD1	1:A:1540:LEU:CD1	2.84	0.55
1:B:1253:SER:CA	1:B:1473:GLN:NE2	2.68	0.55
1:B:1340:TRP:O	1:B:1343:GLN:HB2	2.06	0.55
1:B:1392:GLU:HG3	1:B:1398:SER:HB2	1.88	0.55
1:A:1200:VAL:HG12	1:A:1201:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:GLN:OE1	1:A:1256:ASN:HA	2.05	0.55
1:B:1603:GLU:O	1:B:1607:ARG:HG3	2.06	0.55
1:A:1290:GLU:HG2	1:A:1291:SER:N	2.20	0.55
1:B:1533:PHE:CD2	1:B:1636:LEU:CD2	2.89	0.55
1:A:1339:ARG:HH11	1:A:1339:ARG:CG	2.16	0.55
1:B:1258:ASP:OD2	1:B:1262:THR:OG1	2.20	0.55
1:A:1202:LEU:HD13	1:A:1353:PHE:CG	2.42	0.55
1:A:1272:ARG:NH1	1:A:1272:ARG:H	2.05	0.55
1:A:1276:THR:HG23	1:A:1279:LYS:CE	2.36	0.55
1:B:1577:GLU:OE1	1:B:1601:HIS:ND1	2.38	0.55
1:A:1207:ASP:OD2	1:A:1209:ARG:NH1	2.39	0.55
1:A:1332:ILE:HG13	1:A:1378:LEU:O	2.06	0.55
1:A:1547:CYS:SG	1:A:1584:ASN:OD1	2.65	0.55
1:B:1485:VAL:O	1:B:1487:PRO:HD3	2.06	0.55
1:A:1392:GLU:HG3	1:A:1398:SER:HB2	1.89	0.55
1:A:1346:GLU:OE1	1:A:1349:LYS:CE	2.55	0.54
1:A:1398:SER:CB	1:A:1464:ILE:HD13	2.33	0.54
1:B:1582:VAL:HG12	1:B:1582:VAL:O	2.06	0.54
1:B:1372:GLY:HA2	1:B:1377:GLN:CG	2.37	0.54
1:A:1223:ARG:NH1	1:B:1578:CYS:SG	2.77	0.54
1:A:1331:ASN:HA	1:A:1377:GLN:NE2	2.22	0.54
1:A:1363:LEU:CD2	1:A:1396:PHE:CE1	2.91	0.54
1:B:1272:ARG:HH11	1:B:1272:ARG:HG2	1.71	0.54
1:B:1561:ILE:HA	1:B:1618:VAL:HG13	1.88	0.54
1:A:1577:GLU:OE1	1:A:1601:HIS:ND1	2.40	0.54
1:B:1214:VAL:CG2	1:B:1454:PHE:CD1	2.90	0.54
1:B:1559:LYS:HE3	1:B:1613:LEU:HB2	1.89	0.54
1:A:1409:GLU:OE2	1:A:1453:ARG:NH2	2.32	0.54
1:B:1502:TRP:CZ2	1:B:1506:LYS:HE2	2.43	0.54
1:A:1527:ILE:CD1	1:A:1533:PHE:HD1	2.18	0.53
1:B:1551:ARG:NH1	1:B:1620:GLU:OE1	2.42	0.53
1:B:1586:LEU:HD12	1:B:1619:LEU:HD12	1.90	0.53
1:A:1215:ILE:HD11	1:A:1461:LEU:H	1.73	0.53
1:A:1225:ASN:HB3	1:A:1228:LEU:HD12	1.90	0.53
1:A:1230:SER:O	1:A:1234:LEU:HG	2.09	0.53
1:A:1415:GLU:HB2	1:A:1467:GLY:HA3	1.90	0.53
1:B:1536:ILE:HG13	1:B:1634:PHE:CE2	2.44	0.53
1:A:1566:ARG:NH1	1:A:1566:ARG:HB3	2.24	0.53
1:B:1333:ASP:O	1:B:1334:LEU:HD23	2.08	0.53
1:B:1582:VAL:CG1	1:B:1586:LEU:HB3	2.36	0.53
1:A:1555:VAL:HG23	1:A:1561:ILE:CD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:LEU:O	1:A:1221:SER:HB3	2.09	0.52
1:A:1577:GLU:CG	1:A:1605:CYS:HB3	2.38	0.52
1:A:1333:ASP:O	1:A:1334:LEU:HD23	2.09	0.52
1:A:1526:LYS:HE3	1:B:1269:GLU:CD	2.34	0.52
1:B:1609:ARG:HG3	1:B:1610:SER:N	2.25	0.52
1:A:1400:ASN:ND2	2:A:1701:OGA:O4	2.42	0.52
1:A:1533:PHE:CZ	1:A:1537:LYS:HD2	2.45	0.52
1:B:1373:MET:SD	1:B:1511:ILE:HG21	2.50	0.52
1:B:1523:ARG:HD3	1:B:1524:THR:HG23	1.92	0.52
1:A:1373:MET:SD	1:A:1511:ILE:CG2	2.97	0.52
1:A:1585:ILE:O	1:A:1586:LEU:HD23	2.09	0.52
1:A:1169:LYS:HB3	1:A:1171:ASN:HD21	1.75	0.52
1:B:1398:SER:CB	1:B:1464:ILE:HD13	2.37	0.52
1:A:1177:PRO:HG2	1:A:1180:LYS:HG2	1.92	0.52
1:A:1258:ASP:OD1	1:A:1261:GLY:CA	2.57	0.52
1:B:1215:ILE:CD1	1:B:1461:LEU:H	2.22	0.52
1:B:1231:THR:OG1	1:B:1380:MET:CE	2.58	0.52
1:B:1366:VAL:HG21	1:B:1370:ILE:HD11	1.91	0.52
1:A:1372:GLY:HA2	1:A:1377:GLN:CG	2.39	0.52
1:A:1561:ILE:HA	1:A:1618:VAL:HG13	1.92	0.51
1:B:1177:PRO:HB2	1:B:1179:GLU:OE2	2.10	0.51
1:B:1563:TYR:CD2	1:B:1563:TYR:O	2.61	0.51
1:B:1420:THR:O	1:B:1423:ALA:HB3	2.10	0.51
1:B:1214:VAL:CG2	1:B:1454:PHE:CE1	2.92	0.51
1:A:1164:GLN:HE22	1:A:1534:LYS:CD	2.24	0.51
1:A:1361:ASN:O	1:A:1364:SER:HB2	2.11	0.51
1:B:1391:GLN:OE1	1:B:1499:ARG:NH1	2.43	0.51
1:B:1431:ASP:OD2	1:B:1434:THR:HG23	2.11	0.51
1:A:1218:LEU:HD22	1:A:1461:LEU:HB2	1.93	0.51
1:A:1231:THR:HG23	1:A:1380:MET:HE1	1.92	0.51
1:A:1252:PRO:HG2	1:A:1255:GLU:CD	2.35	0.51
1:A:1328:PHE:CD1	1:A:1385:SER:HB3	2.46	0.51
1:B:1257:TRP:CE3	1:B:1264:GLN:HG3	2.46	0.51
1:A:1272:ARG:HH11	1:A:1272:ARG:CG	2.23	0.51
1:A:1609:ARG:HG3	1:A:1610:SER:N	2.25	0.51
1:B:1225:ASN:HB3	1:B:1228:LEU:HD12	1.93	0.51
1:B:1401:ILE:HG12	1:B:1461:LEU:HD12	1.93	0.51
1:A:1266:TRP:NE1	1:A:1440:ILE:HD12	2.26	0.50
1:B:1280:TYR:C	1:B:1280:TYR:CD2	2.88	0.50
1:B:1401:ILE:CG1	1:B:1461:LEU:HD12	2.42	0.50
1:B:1402:ASN:OD1	1:B:1404:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1194:ARG:HB2	1:B:1194:ARG:NH2	2.26	0.50
1:B:1272:ARG:NH1	1:B:1272:ARG:CG	2.69	0.50
1:A:1353:PHE:CZ	1:A:1354:MET:HE2	2.46	0.50
1:B:1527:ILE:HD11	1:B:1636:LEU:HA	1.92	0.50
1:A:1214:VAL:CG2	1:A:1454:PHE:CE1	2.92	0.50
1:A:1391:GLN:OE1	1:A:1499:ARG:NH1	2.45	0.50
1:B:1241:HIS:HB3	1:B:1277:ILE:CD1	2.41	0.50
1:A:1536:ILE:HG13	1:A:1634:PHE:CE2	2.46	0.50
1:A:1563:TYR:CZ	1:A:1565:GLY:HA2	2.47	0.50
1:B:1361:ASN:C	1:B:1361:ASN:OD1	2.54	0.50
1:B:1175:LYS:HA	1:B:1448:ASN:HD21	1.76	0.50
1:B:1577:GLU:CG	1:B:1605:CYS:HB3	2.41	0.50
1:A:1345:GLN:NE2	1:B:1506:LYS:NZ	2.59	0.50
1:B:1587:PHE:O	1:B:1600:VAL:HA	2.12	0.50
1:A:1252:PRO:HG2	1:A:1255:GLU:OE1	2.12	0.50
1:B:1563:TYR:CD1	1:B:1623:ARG:CD	2.95	0.50
1:B:1176:LEU:HD23	1:B:1180:LYS:HB3	1.93	0.49
1:B:1200:VAL:HG12	1:B:1201:LEU:N	2.27	0.49
1:B:1363:LEU:CD2	1:B:1396:PHE:CE1	2.95	0.49
1:B:1258:ASP:OD1	1:B:1261:GLY:CA	2.59	0.49
1:A:1229:PHE:HB2	1:A:1403:ILE:HD12	1.95	0.49
1:A:1440:ILE:HG22	1:A:1443:ASP:H	1.77	0.49
1:A:1164:GLN:HE22	1:A:1534:LYS:CG	2.23	0.49
1:B:1218:LEU:HD22	1:B:1461:LEU:HB2	1.93	0.49
1:B:1252:PRO:HB2	1:B:1255:GLU:HG2	1.94	0.49
1:B:1256:ASN:O	1:B:1264:GLN:HG2	2.12	0.49
1:A:1188:ILE:O	1:A:1188:ILE:HG22	2.09	0.49
1:B:1328:PHE:CD1	1:B:1385:SER:HB3	2.47	0.49
1:A:1255:GLU:CB	1:A:1257:TRP:HE1	2.24	0.49
1:B:1231:THR:HG23	1:B:1380:MET:HE1	1.94	0.49
1:B:1506:LYS:HB3	1:B:1508:VAL:HG23	1.94	0.49
1:A:1565:GLY:O	1:A:1566:ARG:HG3	2.12	0.49
1:A:1625:GLU:O	1:A:1626:GLU:C	2.55	0.49
1:B:1250:GLN:OE1	1:B:1324:HIS:ND1	2.46	0.49
1:B:1566:ARG:HH11	1:B:1570:GLU:HG2	1.67	0.49
1:A:1193:LYS:HE3	1:B:1577:GLU:O	2.13	0.48
1:B:1529:ASP:OD2	1:B:1532:LEU:N	2.32	0.48
1:A:1193:LYS:NZ	1:B:1578:CYS:CB	2.76	0.48
1:A:1267:PRO:HG3	1:A:1430:VAL:HG21	1.94	0.48
1:B:1566:ARG:HA	1:B:1570:GLU:OE1	2.13	0.48
1:B:1588:VAL:CG1	1:B:1598:TYR:CD1	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1577:GLU:N	1:A:1577:GLU:CD	2.70	0.48
1:B:1231:THR:CG2	1:B:1281:ALA:HB1	2.42	0.48
1:A:1520:ASN:O	1:A:1524:THR:OG1	2.31	0.48
1:A:1378:LEU:HG	1:A:1379:TYR:N	2.28	0.48
1:A:1190:LEU:O	1:B:1608:ARG:NH2	2.47	0.48
1:A:1222:LEU:CB	1:A:1224:LEU:HD12	2.43	0.48
1:A:1551:ARG:NH1	1:A:1620:GLU:OE1	2.46	0.48
1:A:1411:PHE:N	1:A:1411:PHE:CD1	2.82	0.48
1:B:1283:TYR:CE2	1:B:1382:VAL:HG11	2.48	0.48
1:A:1280:TYR:CD2	1:A:1280:TYR:O	2.67	0.48
1:A:1403:ILE:HB	1:A:1479:ASN:O	2.14	0.48
1:A:1526:LYS:HB3	1:A:1637:ALA:CB	2.44	0.48
1:B:1176:LEU:HD22	1:B:1181:LEU:HD23	1.96	0.48
1:A:1207:ASP:OD1	1:A:1208:PRO:HD2	2.13	0.48
1:A:1584:ASN:O	1:A:1586:LEU:HG	2.13	0.48
1:B:1415:GLU:HB2	1:B:1467:GLY:HA3	1.96	0.48
1:B:1222:LEU:CB	1:B:1224:LEU:HD12	2.44	0.47
1:A:1258:ASP:OD2	1:A:1262:THR:OG1	2.32	0.47
1:A:1567:VAL:HG23	1:A:1570:GLU:HB2	1.95	0.47
1:B:1241:HIS:HB3	1:B:1277:ILE:HD12	1.95	0.47
1:B:1258:ASP:OD1	1:B:1262:THR:N	2.44	0.47
1:B:1566:ARG:NH1	1:B:1570:GLU:CD	2.72	0.47
1:A:1272:ARG:N	1:A:1272:ARG:HH11	2.09	0.47
1:B:1472:VAL:HG12	1:B:1473:GLN:N	2.29	0.47
1:A:1178:ARG:C	1:A:1178:ARG:CD	2.88	0.47
1:A:1253:SER:O	1:A:1438:TRP:HZ2	1.98	0.47
1:A:1523:ARG:HB2	1:B:1260:THR:HG23	1.95	0.47
1:A:1178:ARG:HD3	1:A:1178:ARG:O	2.13	0.47
1:A:1257:TRP:CE2	1:A:1264:GLN:HG3	2.50	0.47
1:A:1372:GLY:CA	1:A:1377:GLN:CG	2.92	0.47
1:B:1363:LEU:HD12	1:B:1484:ASN:O	2.14	0.47
1:B:1472:VAL:HG21	2:B:1701:OGA:H4C2	1.95	0.47
1:A:1215:ILE:HG12	1:A:1218:LEU:HD13	1.97	0.47
1:A:1361:ASN:HD21	1:A:1485:VAL:HA	1.78	0.47
1:B:1411:PHE:CD1	1:B:1411:PHE:N	2.83	0.47
1:A:1190:LEU:HD23	1:A:1190:LEU:HA	1.65	0.47
1:A:1363:LEU:HD12	1:A:1484:ASN:O	2.15	0.47
1:A:1566:ARG:NH1	1:A:1566:ARG:CB	2.78	0.47
1:B:1255:GLU:HB3	1:B:1264:GLN:OE1	2.15	0.47
1:B:1351:PRO:HG2	1:B:1354:MET:CE	2.45	0.47
1:A:1253:SER:O	1:A:1438:TRP:CZ2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:THR:O	1:A:1423:ALA:HB3	2.15	0.47
1:A:1587:PHE:O	1:A:1600:VAL:HA	2.15	0.47
1:A:1193:LYS:NZ	1:B:1578:CYS:HB2	2.29	0.47
1:A:1252:PRO:HB2	1:A:1255:GLU:HG2	1.96	0.47
1:A:1275:THR:OG1	1:A:1279:LYS:HD2	2.15	0.47
1:A:1431:ASP:OD2	1:A:1434:THR:HG23	2.15	0.47
1:A:1570:GLU:HA	1:A:1571:PRO:HD2	1.80	0.47
1:B:1266:TRP:NE1	1:B:1440:ILE:HD12	2.30	0.47
1:A:1253:SER:HB2	1:A:1411:PHE:CZ	2.49	0.46
1:A:1276:THR:HG1	1:A:1279:LYS:HG3	1.80	0.46
1:A:1527:ILE:HD13	1:A:1533:PHE:CD1	2.49	0.46
1:B:1563:TYR:CE1	1:B:1623:ARG:NE	2.82	0.46
1:B:1555:VAL:HG23	1:B:1561:ILE:CD1	2.38	0.46
1:A:1529:ASP:OD2	1:A:1532:LEU:HB2	2.14	0.46
1:A:1523:ARG:O	1:B:1259:LEU:HG	2.16	0.46
1:B:1222:LEU:HB2	1:B:1224:LEU:CD1	2.45	0.46
1:B:1272:ARG:HH11	1:B:1272:ARG:N	2.07	0.46
1:B:1188:ILE:O	1:B:1188:ILE:HG22	2.15	0.46
1:B:1225:ASN:O	1:B:1228:LEU:HD12	2.15	0.46
1:A:1373:MET:SD	1:A:1511:ILE:HG21	2.55	0.46
1:A:1222:LEU:HB2	1:A:1224:LEU:CD1	2.45	0.46
1:A:1504:GLU:HG2	1:A:1580:VAL:HG23	1.98	0.46
1:A:1583:PHE:CD2	1:A:1584:ASN:HB2	2.50	0.46
1:A:1160:LEU:CD2	1:A:1497:LEU:CD2	2.89	0.46
1:A:1185:THR:HG21	1:A:1454:PHE:HB3	1.98	0.46
1:A:1566:ARG:NH1	1:A:1570:GLU:OE1	2.49	0.46
1:B:1160:LEU:CD2	1:B:1497:LEU:CD2	2.90	0.46
1:A:1330:THR:O	1:A:1331:ASN:HB2	2.15	0.46
1:B:1243:VAL:HG12	1:B:1277:ILE:CG1	2.46	0.46
1:B:1253:SER:O	1:B:1438:TRP:CZ2	2.69	0.46
1:B:1625:GLU:O	1:B:1626:GLU:C	2.57	0.46
1:A:1258:ASP:OD1	1:A:1262:THR:N	2.48	0.45
1:A:1373:MET:CE	1:A:1393:ASN:HB2	2.46	0.45
1:A:1564:GLN:O	1:A:1621:GLN:HA	2.16	0.45
1:B:1243:VAL:HG12	1:B:1277:ILE:HG12	1.98	0.45
1:B:1559:LYS:HD3	1:B:1559:LYS:HA	1.80	0.45
1:A:1176:LEU:HB3	1:A:1180:LYS:HB2	1.99	0.45
1:B:1185:THR:HG21	1:B:1454:PHE:HB3	1.98	0.45
1:B:1176:LEU:N	1:B:1176:LEU:CD1	2.78	0.45
1:B:1257:TRP:CD2	1:B:1264:GLN:HG3	2.51	0.45
1:A:1447:SER:CB	1:A:1449:ILE:HG13	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:ARG:HD2	1:B:1258:ASP:OD2	2.16	0.45
1:B:1372:GLY:CA	1:B:1377:GLN:CG	2.94	0.45
1:B:1449:ILE:HA	1:B:1450:PRO:HD3	1.83	0.45
1:B:1566:ARG:HD2	1:B:1622:TYR:CZ	2.51	0.45
1:A:1257:TRP:CZ3	1:A:1264:GLN:HG3	2.51	0.45
1:B:1222:LEU:HB2	1:B:1224:LEU:HD12	1.98	0.45
1:B:1361:ASN:O	1:B:1364:SER:HB2	2.17	0.45
1:B:1383:PRO:HD3	1:B:1477:TRP:CE2	2.52	0.45
1:B:1454:PHE:HE1	1:B:1462:VAL:HG22	1.80	0.45
1:B:1575:CYS:SG	1:B:1577:GLU:HG2	2.56	0.45
1:A:1339:ARG:NH1	1:A:1339:ARG:CG	2.75	0.45
1:A:1511:ILE:HA	1:A:1511:ILE:HD13	1.34	0.45
1:A:1519:TRP:CE2	1:A:1540:LEU:CD2	2.98	0.45
1:A:1529:ASP:OD2	1:A:1532:LEU:N	2.35	0.45
1:B:1201:LEU:HD12	1:B:1202:LEU:N	2.32	0.45
1:B:1457:ARG:O	1:B:1460:ASP:HB2	2.17	0.45
1:B:1566:ARG:HD3	1:B:1622:TYR:OH	2.16	0.45
1:A:1170:ILE:C	1:A:1172:THR:H	2.25	0.45
1:A:1383:PRO:HD3	1:A:1477:TRP:CE2	2.52	0.45
1:A:1402:ASN:OD1	1:A:1404:GLY:N	2.50	0.45
1:A:1588:VAL:CG1	1:A:1598:TYR:HD1	2.29	0.45
1:B:1253:SER:O	1:B:1438:TRP:HZ2	2.00	0.45
1:B:1381:LYS:CD	1:B:1474:ALA:HB2	2.46	0.45
1:B:1381:LYS:HD2	1:B:1474:ALA:HB2	1.99	0.45
1:B:1589:THR:O	1:B:1598:TYR:HA	2.17	0.45
1:A:1283:TYR:CE2	1:A:1382:VAL:HG11	2.52	0.45
1:A:1440:ILE:O	1:A:1443:ASP:HB2	2.16	0.45
1:A:1441:LEU:HB3	1:A:1445:TYR:CE2	2.52	0.45
1:A:1231:THR:OG1	1:A:1380:MET:HE3	2.18	0.44
1:A:1401:ILE:CG1	1:A:1461:LEU:HD12	2.47	0.44
1:B:1255:GLU:HB2	1:B:1257:TRP:HE1	1.81	0.44
1:B:1577:GLU:N	1:B:1577:GLU:CD	2.75	0.44
1:A:1492:GLN:HE21	1:A:1492:GLN:C	2.22	0.44
1:A:1526:LYS:HB3	1:A:1637:ALA:HB2	2.00	0.44
1:A:1565:GLY:C	1:A:1566:ARG:HG3	2.42	0.44
1:B:1253:SER:HB2	1:B:1411:PHE:CZ	2.49	0.44
1:B:1597:THR:O	1:B:1597:THR:HG22	2.16	0.44
1:A:1500:TYR:CD1	1:A:1514:MET:HB2	2.51	0.44
1:A:1536:ILE:HG13	1:A:1634:PHE:HE2	1.83	0.44
1:A:1166:VAL:HG21	1:A:1490:ALA:HB3	2.00	0.44
1:B:1207:ASP:OD1	1:B:1208:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:THR:OG1	1:A:1262:THR:OG1	2.30	0.44
1:A:1485:VAL:O	1:A:1485:VAL:HG23	2.18	0.44
1:A:1554:LEU:HD23	1:A:1554:LEU:HA	1.71	0.44
1:A:1585:ILE:H	1:A:1585:ILE:HG13	1.62	0.44
1:B:1542:GLN:O	1:B:1546[A]:HIS:CD2	2.71	0.44
1:B:1190:LEU:HD23	1:B:1190:LEU:HA	1.62	0.44
1:A:1529:ASP:OD2	1:A:1532:LEU:CB	2.65	0.44
1:A:1566:ARG:HH11	1:A:1566:ARG:CB	2.31	0.44
1:A:1582:VAL:HG11	1:A:1586:LEU:HD22	1.98	0.44
1:A:1222:LEU:HB2	1:A:1224:LEU:HD12	1.98	0.44
1:A:1244:GLU:OE2	1:A:1331:ASN:OD1	2.36	0.44
1:A:1370:ILE:CG2	1:A:1511:ILE:HG23	2.45	0.44
1:B:1331:ASN:CA	1:B:1377:GLN:NE2	2.79	0.44
1:A:1160:LEU:HG	1:A:1497:LEU:CD2	2.35	0.43
1:A:1568:LYS:HE3	1:A:1568:LYS:HB3	1.76	0.43
1:B:1563:TYR:C	1:B:1563:TYR:HD2	2.14	0.43
1:A:1372:GLY:CA	1:A:1377:GLN:HG2	2.47	0.43
1:A:1454:PHE:HE1	1:A:1462:VAL:HG22	1.83	0.43
1:A:1521:VAL:O	1:A:1522:ALA:C	2.61	0.43
1:A:1276:THR:H	1:A:1279:LYS:HE3	1.82	0.43
1:B:1511:ILE:HA	1:B:1511:ILE:HD13	1.42	0.43
1:A:1161:SER:HB3	1:A:1164:GLN:HG3	2.01	0.43
1:B:1215:ILE:HD11	1:B:1461:LEU:H	1.82	0.43
1:A:1567:VAL:O	1:B:1263:ARG:NH1	2.46	0.43
1:B:1492:GLN:CA	1:B:1492:GLN:NE2	2.81	0.43
1:B:1598:TYR:C	1:B:1599:LEU:HD13	2.43	0.43
1:B:1506:LYS:HD3	1:B:1506:LYS:HA	1.82	0.43
1:A:1225:ASN:O	1:A:1228:LEU:HD12	2.18	0.43
1:A:1415:GLU:HB2	1:A:1467:GLY:C	2.44	0.43
1:B:1544:MET:HE1	1:B:1631:TYR:CD1	2.54	0.43
1:A:1183:PRO:HD2	1:A:1451:VAL:O	2.19	0.43
1:A:1210:ASN:HA	1:A:1211:PRO:HD2	1.87	0.43
1:B:1245:VAL:HG11	1:B:1327:LYS:HE2	2.01	0.43
1:A:1176:LEU:HB3	1:A:1180:LYS:CG	2.49	0.42
1:A:1536:ILE:HD12	1:A:1537:LYS:N	2.30	0.42
1:B:1161:SER:HB3	1:B:1164:GLN:HG3	2.00	0.42
1:B:1519:TRP:CD2	1:B:1540:LEU:CD2	3.00	0.42
1:B:1554:LEU:CD1	1:B:1618:VAL:HG21	2.49	0.42
1:B:1215:ILE:HD13	1:B:1218:LEU:HB2	1.96	0.42
1:A:1202:LEU:HD13	1:A:1353:PHE:CD2	2.54	0.42
1:B:1378:LEU:HG	1:B:1379:TYR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:LYS:O	1:A:1282:GLN:CB	2.67	0.42
1:A:1457:ARG:O	1:A:1460:ASP:HB2	2.18	0.42
1:A:1565:GLY:O	1:A:1566:ARG:HG2	2.18	0.42
1:B:1164:GLN:HE22	1:B:1534:LYS:CG	2.18	0.42
1:B:1410:TRP:O	1:B:1453:ARG:HA	2.20	0.42
1:B:1504:GLU:HG2	1:B:1580:VAL:HG23	2.02	0.42
1:A:1193:LYS:H	1:A:1193:LYS:HG2	1.68	0.42
1:A:1215:ILE:HD13	1:A:1218:LEU:HB2	1.96	0.42
1:A:1349:LYS:HD3	1:B:1507:ASN:OD1	2.19	0.42
1:B:1193:LYS:O	1:B:1196:ALA:N	2.52	0.42
1:B:1373:MET:HA	1:B:1484:ASN:HB2	2.00	0.42
1:B:1275:THR:HG23	1:B:1276:THR:N	2.35	0.42
1:A:1257:TRP:CE2	1:A:1264:GLN:CG	3.02	0.42
1:A:1563:TYR:CE1	1:A:1623:ARG:HG2	2.55	0.42
1:B:1215:ILE:CD1	1:B:1218:LEU:HB2	2.47	0.42
1:B:1440:ILE:O	1:B:1443:ASP:HB2	2.20	0.42
1:A:1505:VAL:HG12	1:A:1506:LYS:N	2.33	0.42
1:A:1410:TRP:O	1:A:1453:ARG:HA	2.20	0.42
1:A:1575:CYS:SG	1:A:1577:GLU:HG2	2.59	0.42
1:B:1193:LYS:O	1:B:1194:ARG:C	2.63	0.42
1:B:1283:TYR:O	1:B:1287:SER:HB3	2.20	0.42
1:B:1527:ILE:HD13	1:B:1533:PHE:CD1	2.51	0.42
1:A:1275:THR:HG23	1:A:1276:THR:N	2.35	0.41
1:B:1215:ILE:HG12	1:B:1218:LEU:HD13	2.02	0.41
1:B:1253:SER:N	1:B:1473:GLN:NE2	2.68	0.41
1:B:1508:VAL:HG12	1:B:1509:LYS:N	2.34	0.41
1:B:1536:ILE:HG13	1:B:1634:PHE:HE2	1.83	0.41
1:B:1402:ASN:HB2	1:B:1456:GLN:OE1	2.20	0.41
1:A:1197:PHE:CE1	1:A:1351:PRO:HA	2.55	0.41
1:A:1201:LEU:C	1:A:1201:LEU:CD1	2.81	0.41
1:A:1272:ARG:NH1	1:A:1272:ARG:CG	2.82	0.41
1:B:1176:LEU:CD1	1:B:1448:ASN:CG	2.93	0.41
1:B:1566:ARG:HG2	1:B:1621:GLN:HB3	2.00	0.41
1:A:1255:GLU:HB2	1:A:1257:TRP:CD1	2.56	0.41
1:A:1356:VAL:HG22	1:A:1483:TRP:CD1	2.56	0.41
1:B:1532:LEU:O	1:B:1536:ILE:HG23	2.20	0.41
1:B:1597:THR:O	1:B:1597:THR:CG2	2.68	0.41
1:A:1542:GLN:O	1:A:1546[A]:HIS:CD2	2.73	0.41
1:B:1183:PRO:HD2	1:B:1451:VAL:O	2.20	0.41
1:B:1441:LEU:HB3	1:B:1445:TYR:CE2	2.55	0.41
1:A:1564:GLN:O	1:A:1565:GLY:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1188:ILE:HD12	1:B:1188:ILE:HA	1.76	0.41
1:B:1369:THR:CG2	1:B:1375:THR:CG2	2.99	0.41
1:A:1373:MET:HA	1:A:1484:ASN:HB2	2.01	0.41
1:B:1243:VAL:HG11	1:B:1277:ILE:CG1	2.44	0.41
1:B:1570:GLU:HA	1:B:1571:PRO:HD2	1.81	0.41
1:A:1255:GLU:HB3	1:A:1264:GLN:OE1	2.20	0.41
1:A:1544:MET:HE1	1:A:1631:TYR:CD1	2.56	0.41
1:B:1177:PRO:CB	1:B:1179:GLU:OE2	2.69	0.41
1:B:1529:ASP:OD2	1:B:1532:LEU:HB2	2.21	0.41
1:A:1256:ASN:O	1:A:1264:GLN:HG2	2.20	0.41
1:A:1257:TRP:CE2	1:A:1264:GLN:CD	2.99	0.41
1:B:1463:TRP:CD1	1:B:1463:TRP:C	2.98	0.41
1:A:1405:PRO:O	1:A:1458:PRO:CG	2.69	0.40
1:B:1214:VAL:HG11	1:B:1216:ARG:NH1	2.37	0.40
1:B:1284:GLN:NE2	1:B:1380:MET:HB3	2.33	0.40
1:B:1339:ARG:HH21	1:B:1339:ARG:HB3	1.83	0.40
1:A:1214:VAL:HG11	1:A:1216:ARG:NH1	2.37	0.40
1:A:1257:TRP:CD2	1:A:1264:GLN:CG	3.01	0.40
1:A:1279:LYS:O	1:A:1282:GLN:HB2	2.21	0.40
1:A:1280:TYR:HE2	1:A:1284:GLN:NE2	2.16	0.40
1:B:1222:LEU:HD23	1:B:1222:LEU:HA	1.84	0.40
1:B:1252:PRO:HG2	1:B:1255:GLU:CD	2.47	0.40
1:B:1492:GLN:NE2	1:B:1492:GLN:HA	2.36	0.40
1:B:1554:LEU:HA	1:B:1554:LEU:HD23	1.74	0.40
1:B:1252:PRO:HB2	1:B:1255:GLU:CG	2.52	0.40
1:B:1369:THR:HG23	1:B:1375:THR:CG2	2.51	0.40
1:B:1601:HIS:HB2	1:B:1606:ALA:HB2	2.04	0.40
1:A:1566:ARG:NH1	1:A:1621:GLN:NE2	2.69	0.40
1:B:1361:ASN:HA	1:B:1486:GLY:O	2.22	0.40
1:B:1519:TRP:CE2	1:B:1540:LEU:CD2	3.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/486 (91%)	420 (95%)	23 (5%)	0	100	100
1	B	440/486 (90%)	421 (96%)	19 (4%)	0	100	100
All	All	883/972 (91%)	841 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/424 (94%)	322 (81%)	76 (19%)	1	8
1	B	396/424 (93%)	324 (82%)	72 (18%)	2	9
All	All	794/848 (94%)	646 (81%)	148 (19%)	1	9

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1157	GLU
1	A	1171	ASN
1	A	1174	GLU
1	A	1176	LEU
1	A	1178	ARG
1	A	1179	GLU
1	A	1181	LEU
1	A	1185	THR
1	A	1188	ILE
1	A	1194	ARG
1	A	1200	VAL
1	A	1201	LEU
1	A	1215	ILE
1	A	1218	LEU
1	A	1224	LEU

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Mol	Chain	Res	Type
1	A	1243	VAL
1	A	1244	GLU
1	A	1249	VAL
1	A	1254	ASP
1	A	1262	THR
1	A	1263	ARG
1	A	1270	SER
1	A	1272	ARG
1	A	1273	SER
1	A	1275	THR
1	A	1287	SER
1	A	1290	GLU
1	A	1292	LEU
1	A	1293	GLN
1	A	1295	GLU
1	A	1325	ILE
1	A	1332	ILE
1	A	1333	ASP
1	A	1338	LYS
1	A	1339	ARG
1	A	1345	GLN
1	A	1370	ILE
1	A	1371	LEU
1	A	1378	LEU
1	A	1411	PHE
1	A	1419	GLU
1	A	1420	THR
1	A	1442	ASP
1	A	1453	ARG
1	A	1455	VAL
1	A	1457	ARG
1	A	1481	ILE
1	A	1497	LEU
1	A	1499	ARG
1	A	1505	VAL
1	A	1506	LYS
1	A	1507	ASN
1	A	1508	VAL
1	A	1511	ILE
1	A	1517	VAL
1	A	1520	ASN
1	A	1523	ARG

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Mol	Chain	Res	Type
1	A	1524	THR
1	A	1525	VAL
1	A	1528	SER
1	A	1534	LYS
1	A	1536	ILE
1	A	1548	GLN
1	A	1552	GLU
1	A	1555	VAL
1	A	1560	LYS
1	A	1561	ILE
1	A	1566	ARG
1	A	1577	GLU
1	A	1584	ASN
1	A	1591	GLU
1	A	1619	LEU
1	A	1624	THR
1	A	1625	GLU
1	A	1632	ASP
1	A	1635	THR
1	B	1157	GLU
1	B	1176	LEU
1	B	1179	GLU
1	B	1181	LEU
1	B	1185	THR
1	B	1188	ILE
1	B	1194	ARG
1	B	1200	VAL
1	B	1201	LEU
1	B	1209	ARG
1	B	1215	ILE
1	B	1218	LEU
1	B	1224	LEU
1	B	1243	VAL
1	B	1246	ARG
1	B	1249	VAL
1	B	1254	ASP
1	B	1263	ARG
1	B	1270	SER
1	B	1272	ARG
1	B	1273	SER
1	B	1275	THR
1	B	1287	SER

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Mol	Chain	Res	Type
1	B	1292	LEU
1	B	1293	GLN
1	B	1325	ILE
1	B	1327	LYS
1	B	1333	ASP
1	B	1338	LYS
1	B	1339	ARG
1	B	1345	GLN
1	B	1370	ILE
1	B	1371	LEU
1	B	1378	LEU
1	B	1408	CYS
1	B	1419	GLU
1	B	1420	THR
1	B	1442	ASP
1	B	1453	ARG
1	B	1455	VAL
1	B	1457	ARG
1	B	1461	LEU
1	B	1481	ILE
1	B	1497	LEU
1	B	1499	ARG
1	B	1511	ILE
1	B	1517	VAL
1	B	1518	SER
1	B	1523	ARG
1	B	1524	THR
1	B	1525	VAL
1	B	1528	SER
1	B	1536	ILE
1	B	1537	LYS
1	B	1548	GLN
1	B	1552	GLU
1	B	1555	VAL
1	B	1560	LYS
1	B	1561	ILE
1	B	1563	TYR
1	B	1564	GLN
1	B	1567	VAL
1	B	1568	LYS
1	B	1577	GLU
1	B	1582	VAL

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Mol	Chain	Res	Type
1	B	1586	LEU
1	B	1599	LEU
1	B	1607	ARG
1	B	1619	LEU
1	B	1624	THR
1	B	1632	ASP
1	B	1635	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1164	GLN
1	A	1171	ASN
1	A	1284	GLN
1	A	1331	ASN
1	A	1345	GLN
1	A	1377	GLN
1	A	1416	HIS
1	A	1473	GLN
1	A	1503	ASN
1	A	1584	ASN
1	A	1621	GLN
1	B	1164	GLN
1	B	1284	GLN
1	B	1377	GLN
1	B	1416	HIS
1	B	1473	GLN
1	B	1507	ASN
1	B	1564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	OGA	B	1701	3	9,9,9	1.17	0	8,11,11	1.06	0
2	OGA	A	1701	3	9,9,9	1.11	0	8,11,11	1.02	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	OGA	B	1701	3	-	0/8/9/9	-
2	OGA	A	1701	3	-	0/8/9/9	-

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1701	OGA	1	0
2	A	1701	OGA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	448/486 (92%)	0.48	25 (5%)	30 15	24, 57, 98, 141	1 (0%)
1	B	447/486 (91%)	0.47	28 (6%)	26 13	26, 57, 100, 148	1 (0%)
All	All	895/972 (92%)	0.48	53 (5%)	28 14	24, 57, 100, 148	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1610	SER	5.7
1	B	1613	LEU	5.6
1	B	1591	GLU	5.6
1	B	1614	GLN	5.3
1	A	1406	GLY	5.2
1	B	1290	GLU	4.8
1	B	1294	GLU	4.2
1	B	1597	THR	4.2
1	A	1174	GLU	4.2
1	A	1613	LEU	4.1
1	B	1253	SER	3.9
1	A	1481	ILE	3.8
1	A	1257	TRP	3.7
1	B	1615	GLY	3.6
1	A	1172	THR	3.6
1	B	1174	GLU	3.5
1	B	1612	GLY	3.4
1	A	1173	GLU	3.2
1	B	1178	ARG	3.0
1	B	1563	TYR	2.9
1	A	1597	THR	2.8
1	B	1406	GLY	2.7
1	A	1504	GLU	2.7
1	A	1585	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1224	LEU	2.7
1	A	1612	GLY	2.6
1	B	1434	THR	2.6
1	A	1253	SER	2.6
1	A	1615	GLY	2.6
1	B	1257	TRP	2.6
1	A	1563	TYR	2.6
1	B	1600	VAL	2.5
1	B	1616	VAL	2.5
1	A	1294	GLU	2.5
1	A	1405	PRO	2.4
1	A	1582	VAL	2.4
1	B	1558	GLY	2.4
1	B	1179	GLU	2.4
1	B	1194	ARG	2.4
1	A	1616	VAL	2.3
1	B	1520	ASN	2.3
1	A	1614	GLN	2.3
1	A	1591	GLU	2.3
1	B	1553	SER	2.3
1	A	1478	CYS	2.2
1	B	1246	ARG	2.2
1	A	1331	ASN	2.2
1	A	1178	ARG	2.1
1	B	1333	ASP	2.1
1	B	1367	GLY	2.1
1	A	1610	SER	2.0
1	A	1171	ASN	2.0
1	B	1277	ILE	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
2	OGA	A	1701	10/10	0.85	0.19	41,60,68,86	0
2	OGA	B	1701	10/10	0.88	0.15	20,20,20,20	0
3	NI	B	1702	1/1	0.97	0.10	41,41,41,41	0
3	NI	A	1702	1/1	0.98	0.09	46,46,46,46	0
4	ZN	A	1703	1/1	0.99	0.03	67,67,67,67	0
4	ZN	B	1703	1/1	0.99	0.04	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.