



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:48 PM UTC

PDB ID : 1IKY / pdb_00001iky
Title : HIV-1 Reverse Transcriptase in Complex with the Inhibitor MSC194
Authors : Lindberg, J.; Unge, T.
Deposited on : 2001-05-07
Resolution : 3.00 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

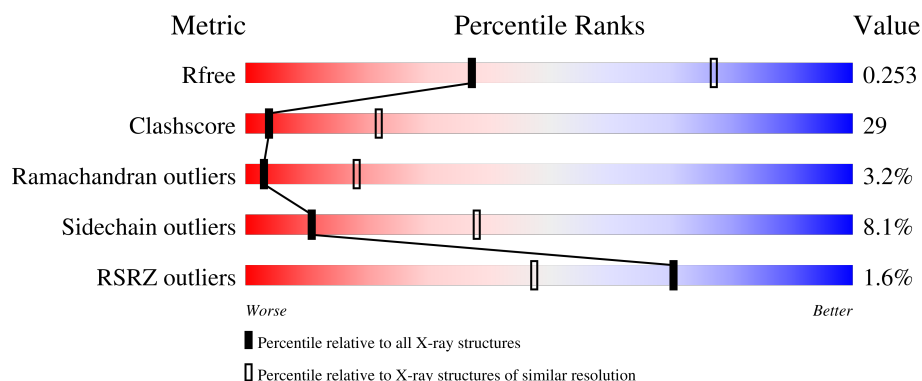
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	560	 48% 43% 8% 3%
2	B	427	 3% 48% 40% 6% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7918 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	2	0	0
			4522	2925	754	835	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	478	GLN	GLU	engineered mutation	UNP P03366

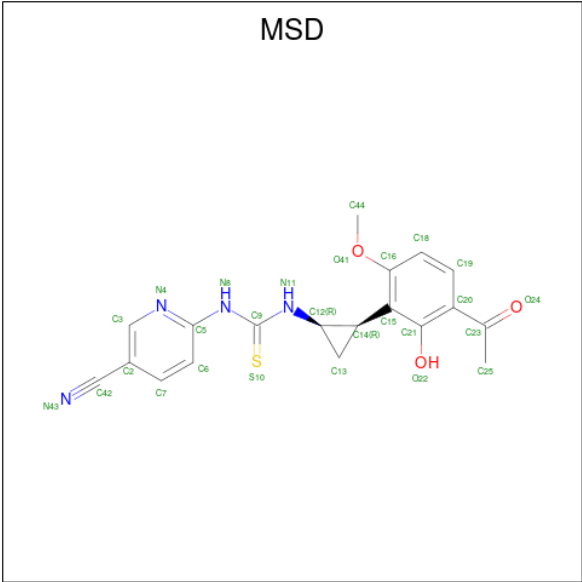
- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	30	0	0
			3345	2178	550	611	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1103	ASN	LYS	engineered mutation	UNP P03366

- Molecule 3 is 1-[2-(3-ACETYL-2-HYDROXY-6-METHOXY-PHENYL)-CYCLOPROPYL]-3-(5-CYANO-PYRIDIN-2-YL)-THIOUREA (CCD ID: MSD) (formula: C₁₉H₁₈N₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	19	4	3	1		

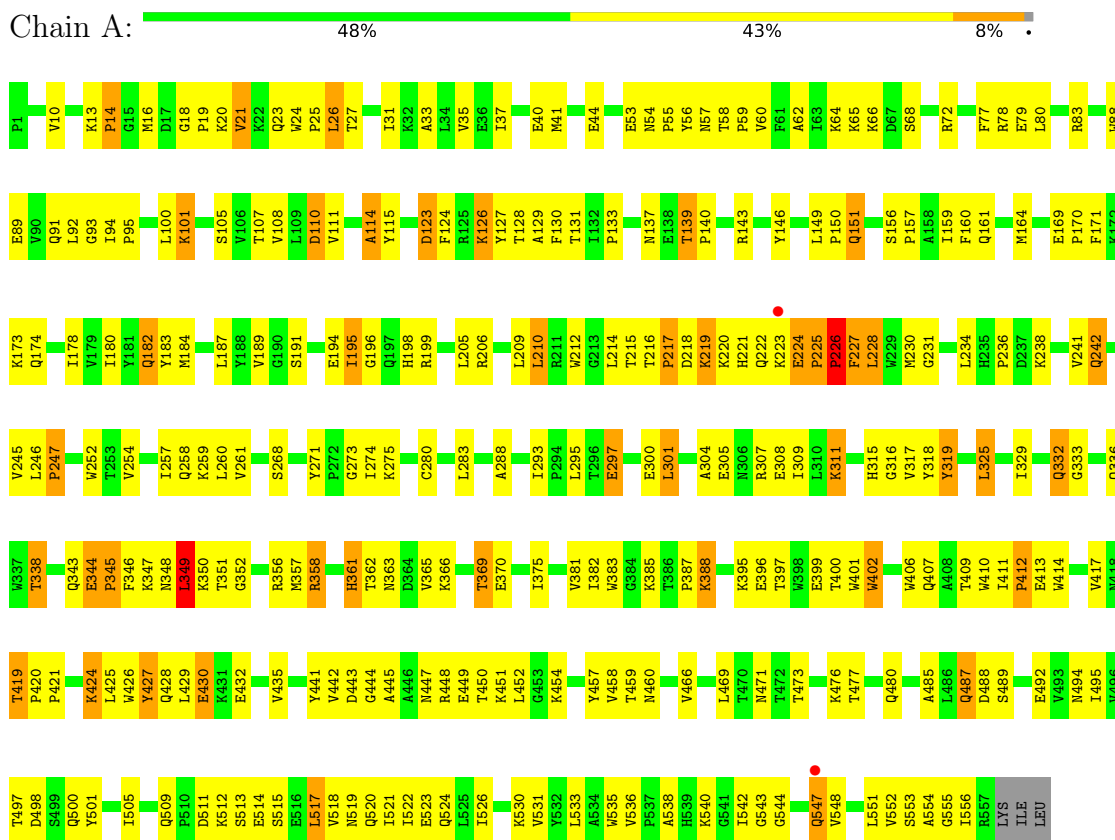
- Molecule 4 is water.

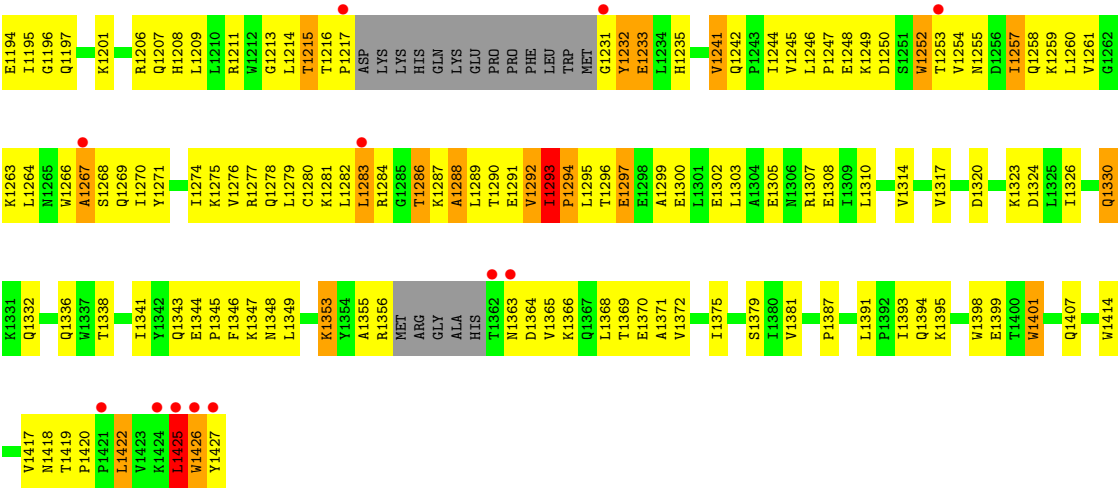
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	16	Total	O	0	0
			16	16		

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: POL POLYPROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.34Å 156.54Å 156.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.78 – 3.00 45.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.8 (45.78-3.00) 90.8 (45.78-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.273 0.198 , 0.253	Depositor DCC
R_{free} test set	1388 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7918	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MSD

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	0.50	0/4640	1.00	21/6305 (0.3%)
2	B	0.48	0/3439	0.99	22/4674 (0.5%)
All	All	0.49	0/8079	0.99	43/10979 (0.4%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	CA-C-N	8.43	130.38	119.84
1	A	13	LYS	C-N-CA	8.43	130.38	119.84
1	A	419	THR	CA-C-N	7.30	127.90	120.38
1	A	419	THR	C-N-CA	7.30	127.90	120.38
2	B	1018	GLY	CA-C-N	7.18	127.62	119.93
2	B	1018	GLY	C-N-CA	7.18	127.62	119.93
1	A	225	PRO	N-CA-C	-7.08	102.06	110.70
1	A	246	LEU	CA-C-N	7.00	128.59	119.84
1	A	246	LEU	C-N-CA	7.00	128.59	119.84
2	B	1245	VAL	N-CA-C	6.57	117.51	109.30
2	B	1401	TRP	N-CA-C	6.38	122.54	114.31
2	B	1235	HIS	CA-C-N	6.29	125.79	119.24
2	B	1235	HIS	C-N-CA	6.29	125.79	119.24
2	B	1175	ASN	CA-C-N	6.24	125.86	119.56
2	B	1175	ASN	C-N-CA	6.24	125.86	119.56
1	A	382	ILE	N-CA-C	6.17	116.64	110.23
2	B	1132	ILE	N-CA-C	-6.15	101.46	107.55
2	B	1103	ASN	N-CA-C	5.95	117.98	110.24
2	B	1112	GLY	N-CA-C	5.91	119.64	112.49
1	A	58	THR	CA-C-N	5.83	126.17	119.93
1	A	58	THR	C-N-CA	5.83	126.17	119.93
2	B	1349	LEU	N-CA-C	-5.72	105.02	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	TYR	N-CA-C	5.63	118.71	109.76
2	B	1194	GLU	N-CA-C	-5.60	102.73	110.35
1	A	242	GLN	N-CA-C	-5.55	103.22	109.60
2	B	1391	LEU	N-CA-C	5.47	116.84	109.24
1	A	349	LEU	N-CA-C	-5.45	104.88	112.45
2	B	1269	GLN	N-CA-C	-5.45	106.47	113.01
1	A	53	GLU	N-CA-C	-5.42	106.71	113.38
1	A	540	LYS	N-CA-C	-5.41	106.72	113.38
2	B	1233	GLU	N-CA-C	5.38	117.67	108.90
2	B	1293	ILE	CA-C-N	5.33	126.50	119.84
2	B	1293	ILE	C-N-CA	5.33	126.50	119.84
1	A	500	GLN	N-CA-C	-5.26	104.80	111.11
1	A	388	LYS	N-CA-C	-5.25	101.13	109.96
2	B	1288	ALA	N-CA-C	-5.19	103.54	110.55
1	A	383	TRP	N-CA-C	5.15	120.20	113.30
1	A	54	ASN	CA-C-N	5.10	125.78	120.12
1	A	54	ASN	C-N-CA	5.10	125.78	120.12
2	B	1208	HIS	N-CA-C	-5.07	105.65	111.07
2	B	1348	ASN	N-CA-C	5.04	117.47	109.96
2	B	1425	LEU	N-CA-C	-5.03	100.88	108.67
1	A	311	LYS	N-CA-C	5.02	116.44	110.97

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	4522	0	4572	260	1
2	B	3345	0	3372	202	0
3	A	27	0	17	4	0
4	A	8	0	0	0	0
4	B	16	0	0	1	0
All	All	7918	0	7961	450	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 29.

All (450) 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:131:THR:HG22	1:A:143:ARG:HG2	1.36	1.03
2:B:1215:THR:HG22	2:B:1216:THR:H	1.24	1.01
1:A:458:VAL:HG21	1:A:547:GLN:HE22	1.32	0.94
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.53	0.90
1:A:435:VAL:HG13	2:B:1290:THR:HG21	1.55	0.89
2:B:1266:TRP:CD1	2:B:1427:TYR:HH	1.90	0.88
2:B:1206:ARG:HG2	2:B:1216:THR:HG21	1.55	0.88
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.56	0.88
1:A:65:LYS:HG3	1:A:66:LYS:H	1.42	0.84
2:B:1283:LEU:HD22	2:B:1293:ILE:HB	1.59	0.84
2:B:1184:MET:O	2:B:1185:ASP:HB2	1.77	0.83
2:B:1314:VAL:O	2:B:1317:VAL:HG22	1.79	0.82
2:B:1060:VAL:HG12	2:B:1075:VAL:HG22	1.61	0.82
1:A:27:THR:O	1:A:31:ILE:HG13	1.80	0.81
1:A:225:PRO:HA	1:A:226:PRO:O	1.82	0.80
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.63	0.78
2:B:1303:LEU:HB3	2:B:1307:ARG:HH12	1.47	0.78
1:A:458:VAL:CG2	1:A:547:GLN:HE22	1.96	0.78
2:B:1280:CYS:HA	2:B:1284:ARG:HH21	1.49	0.78
1:A:178:ILE:HD13	1:A:191:SER:HB3	1.67	0.77
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.67	0.77
2:B:1280:CYS:HA	2:B:1284:ARG:NH2	2.00	0.76
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.14	0.76
2:B:1063:ILE:HD13	2:B:1074:LEU:HD22	1.66	0.75
1:A:89:GLU:HB2	1:A:92:LEU:HD11	1.68	0.75
1:A:64:LYS:HD3	1:A:68:SER:HB3	1.67	0.74
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.68	0.73
2:B:1154:LYS:HG2	2:B:1184:MET:HE2	1.71	0.73
1:A:206:ARG:HE	1:A:216:THR:HG23	1.54	0.72
2:B:1215:THR:HG22	2:B:1216:THR:N	2.03	0.72
1:A:466:VAL:HG21	1:A:551:LEU:HD13	1.71	0.71
2:B:1253:THR:O	2:B:1257:ILE:HG22	1.90	0.71
2:B:1332:GLN:HB2	2:B:1336:GLN:HB2	1.71	0.71
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.54	0.71
1:A:450:THR:O	1:A:451:LYS:HB2	1.90	0.71
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.73	0.70
1:A:107:THR:HB	1:A:223:LYS:HB3	1.74	0.70
2:B:1282:LEU:HB3	2:B:1283:LEU:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1287:LYS:HD3	2:B:1291:GLU:OE2	1.91	0.69
2:B:1279:LEU:HD12	2:B:1282:LEU:HD22	1.74	0.69
2:B:1296:THR:O	2:B:1300:GLU:HG2	1.93	0.69
1:A:254:VAL:O	1:A:258:GLN:HG3	1.93	0.69
2:B:1417:VAL:HG22	2:B:1418:ASN:H	1.59	0.68
1:A:458:VAL:HG11	1:A:547:GLN:CD	2.17	0.68
1:A:458:VAL:HG21	1:A:547:GLN:NE2	2.08	0.68
1:A:458:VAL:HG11	1:A:547:GLN:OE1	1.93	0.68
2:B:1050:ILE:CG2	2:B:1145:GLN:HG2	2.23	0.68
2:B:1195:ILE:HG23	2:B:1196:GLY:N	2.08	0.68
2:B:1355:ALA:O	2:B:1356:ARG:HB2	1.94	0.68
2:B:1420:PRO:C	2:B:1422:LEU:H	2.01	0.68
1:A:396:GLU:O	1:A:400:THR:HG22	1.94	0.67
2:B:1090:VAL:HG23	2:B:1091:GLN:N	2.08	0.67
1:A:93:GLY:O	1:A:94:ILE:HD13	1.94	0.67
1:A:458:VAL:HG23	1:A:548:VAL:HG13	1.76	0.67
2:B:1283:LEU:CD2	2:B:1293:ILE:HB	2.24	0.67
2:B:1283:LEU:HD22	2:B:1293:ILE:CB	2.24	0.67
1:A:305:GLU:O	1:A:309:ILE:HG13	1.95	0.66
1:A:275:LYS:HG2	1:A:336:GLN:HE22	1.58	0.66
1:A:457:TYR:CD1	1:A:457:TYR:C	2.74	0.66
2:B:1275:LYS:HE3	2:B:1277:ARG:HB3	1.77	0.66
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.31	0.66
2:B:1369:THR:HG22	2:B:1398:TRP:CH2	2.31	0.66
1:A:450:THR:HG21	1:A:452:LEU:HD12	1.76	0.66
2:B:1209:LEU:HD22	2:B:1214:LEU:HD23	1.77	0.66
1:A:101:LYS:HE3	1:A:101:LYS:N	2.11	0.65
1:A:219:LYS:CD	1:A:220:LYS:HG2	2.26	0.65
1:A:357:MET:HG3	1:A:358:ARG:H	1.62	0.65
1:A:62:ALA:HA	1:A:72:ARG:O	1.96	0.65
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.27	0.65
1:A:107:THR:HG23	1:A:198:HIS:NE2	2.12	0.65
1:A:223:LYS:HG3	1:A:224:GLU:N	2.13	0.64
1:A:301:LEU:O	1:A:304:ALA:HB3	1.97	0.64
1:A:402:TRP:CD1	1:A:402:TRP:C	2.75	0.64
2:B:1007:THR:HG22	2:B:1119:PRO:HG2	1.78	0.64
2:B:1139:THR:HG23	2:B:1140:PRO:HD2	1.79	0.63
2:B:1280:CYS:CA	2:B:1284:ARG:HH21	2.11	0.63
2:B:1114:ALA:HB2	2:B:1214:LEU:HD11	1.79	0.63
1:A:101:LYS:HE3	1:A:101:LYS:H	1.63	0.63
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.28	0.63
1:A:441:TYR:O	1:A:548:VAL:HG21	1.99	0.63
2:B:1059:PRO:HG2	2:B:1076:ASP:HB3	1.80	0.63
2:B:1282:LEU:C	2:B:1283:LEU:HD12	2.24	0.62
1:A:234:LEU:HD12	1:A:234:LEU:N	2.14	0.62
1:A:420:PRO:HA	1:A:421:PRO:C	2.23	0.62
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.34	0.62
2:B:1279:LEU:O	2:B:1282:LEU:HB2	1.98	0.62
2:B:1050:ILE:HG21	2:B:1145:GLN:HG2	1.82	0.62
1:A:89:GLU:HB2	1:A:92:LEU:CD1	2.30	0.61
1:A:223:LYS:HG3	1:A:224:GLU:H	1.66	0.61
2:B:1252:TRP:HA	2:B:1252:TRP:CE3	2.35	0.61
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.27	0.61
2:B:1091:GLN:O	2:B:1092:LEU:HD23	2.00	0.61
2:B:1257:ILE:O	2:B:1261:VAL:HG23	1.99	0.61
1:A:65:LYS:HG3	1:A:66:LYS:N	2.15	0.61
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.65	0.61
2:B:1252:TRP:HA	2:B:1252:TRP:HE3	1.66	0.60
1:A:219:LYS:HD2	1:A:220:LYS:HG2	1.82	0.60
1:A:547:GLN:NE2	1:A:548:VAL:N	2.50	0.60
1:A:268:SER:O	1:A:351:THR:HG22	2.01	0.60
2:B:1090:VAL:CG2	2:B:1091:GLN:N	2.64	0.60
2:B:1303:LEU:HB3	2:B:1307:ARG:NH1	2.16	0.60
1:A:447:ASN:OD1	1:A:449:GLU:HG2	2.02	0.60
1:A:64:LYS:HB3	1:A:68:SER:HA	1.83	0.60
1:A:228:LEU:N	1:A:228:LEU:HD23	2.16	0.60
1:A:332:GLN:HG3	1:A:338:THR:HG22	1.84	0.59
1:A:458:VAL:CB	1:A:547:GLN:HE22	2.15	0.59
2:B:1422:LEU:HD23	2:B:1422:LEU:O	2.00	0.59
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.83	0.59
1:A:219:LYS:HD2	1:A:219:LYS:H	1.66	0.59
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.84	0.59
2:B:1191:SER:HB2	2:B:1193:LEU:HD13	1.85	0.58
2:B:1231:GLY:O	2:B:1232:TYR:HB3	2.02	0.58
2:B:1320:ASP:OD2	2:B:1323:LYS:HG3	2.04	0.58
1:A:427:TYR:O	1:A:509:GLN:NE2	2.37	0.58
2:B:1160:PHE:HE2	2:B:1164:MET:HE2	1.69	0.58
2:B:1215:THR:O	2:B:1216:THR:HG23	2.03	0.58
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.03	0.58
1:A:308:GLU:O	1:A:311:LYS:HG2	2.04	0.58
1:A:429:LEU:O	1:A:430:GLU:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1246:LEU:HD12	2:B:1307:ARG:HB3	1.85	0.57
2:B:1254:VAL:O	2:B:1257:ILE:HG23	2.04	0.57
1:A:238:LYS:HB2	1:A:316:GLY:O	2.04	0.57
2:B:1122:GLU:CD	2:B:1122:GLU:H	2.10	0.57
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.87	0.57
1:A:20:LYS:HG2	1:A:55:PRO:O	2.05	0.57
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.87	0.57
2:B:1063:ILE:HD13	2:B:1074:LEU:CD2	2.32	0.57
1:A:411:ILE:O	1:A:411:ILE:HG23	2.04	0.57
2:B:1072:ARG:HD3	2:B:1073:LYS:O	2.05	0.57
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.19	0.57
1:A:428:GLN:HA	1:A:509:GLN:NE2	2.20	0.56
1:A:454:LYS:O	1:A:552:VAL:HG13	2.04	0.56
1:A:543:GLY:H	2:B:1284:ARG:HD2	1.69	0.56
2:B:1280:CYS:C	2:B:1282:LEU:H	2.11	0.56
2:B:1344:GLU:O	2:B:1347:LYS:HB2	2.05	0.56
1:A:231:GLY:C	1:A:242:GLN:HG2	2.29	0.56
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.68	0.56
2:B:1086:ASP:O	2:B:1090:VAL:HG22	2.04	0.56
2:B:1153:TRP:CE2	2:B:1155:GLY:HA3	2.40	0.56
1:A:410:TRP:HB2	2:B:1365:VAL:HG23	1.87	0.56
1:A:33:ALA:O	1:A:37:ILE:HG13	2.06	0.56
1:A:238:LYS:HD2	1:A:315:HIS:CB	2.35	0.56
2:B:1266:TRP:HE1	2:B:1346:PHE:HE2	1.53	0.56
1:A:397:THR:HG21	1:A:424:LYS:HA	1.88	0.56
1:A:131:THR:CG2	1:A:143:ARG:HH11	2.19	0.56
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.87	0.56
1:A:443:ASP:OD1	1:A:444:GLY:N	2.39	0.56
2:B:1271:TYR:O	2:B:1274:ILE:HG12	2.05	0.56
1:A:445:ALA:O	1:A:477:THR:HG21	2.06	0.55
1:A:547:GLN:HE21	1:A:548:VAL:N	2.03	0.55
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.21	0.55
1:A:513:SER:OG	1:A:514:GLU:N	2.40	0.55
2:B:1090:VAL:CG2	2:B:1091:GLN:H	2.20	0.55
2:B:1193:LEU:HB3	2:B:1197:GLN:HB3	1.88	0.55
1:A:37:ILE:HG22	1:A:41:MET:HE3	1.88	0.55
1:A:228:LEU:HB3	1:A:242:GLN:HE22	1.72	0.55
1:A:518:VAL:O	1:A:522:ILE:HG13	2.07	0.55
2:B:1241:VAL:HG12	2:B:1242:GLN:H	1.72	0.55
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.06	0.55
1:A:317:VAL:HG22	1:A:318:TYR:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.89	0.54
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.89	0.54
3:A:2000:MSD:H132	3:A:2000:MSD:O22	2.07	0.54
2:B:1286:THR:HG22	2:B:1286:THR:O	2.08	0.54
1:A:91:GLN:HE22	1:A:183:TYR:HD1	1.55	0.54
1:A:65:LYS:NZ	1:A:72:ARG:HD2	2.22	0.54
1:A:219:LYS:HD2	1:A:220:LYS:N	2.23	0.54
2:B:1085:GLN:HA	2:B:1088:TRP:CE2	2.43	0.54
2:B:1244:ILE:HD13	2:B:1427:TYR:CD2	2.43	0.54
2:B:1066:LYS:O	2:B:1067:ASP:HB2	2.08	0.54
2:B:1085:GLN:O	2:B:1086:ASP:C	2.51	0.54
1:A:219:LYS:HD3	1:A:220:LYS:HG2	1.90	0.53
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.43	0.53
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.89	0.53
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.89	0.53
2:B:1249:LYS:HB3	2:B:1252:TRP:CZ3	2.43	0.53
1:A:317:VAL:HG12	1:A:348:ASN:O	2.09	0.53
1:A:128:THR:OG1	1:A:146:TYR:HB2	2.09	0.53
1:A:227:PHE:C	1:A:228:LEU:HD23	2.33	0.53
2:B:1060:VAL:CG1	2:B:1075:VAL:HG22	2.35	0.53
1:A:458:VAL:CB	1:A:548:VAL:HG22	2.36	0.53
2:B:1195:ILE:HG23	2:B:1196:GLY:H	1.73	0.52
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.73	0.52
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.39	0.52
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.90	0.52
2:B:1077:PHE:HD2	2:B:1152:GLY:HA3	1.74	0.52
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.92	0.52
1:A:225:PRO:HA	1:A:226:PRO:C	2.33	0.52
1:A:426:TRP:O	1:A:427:TYR:HB3	2.10	0.52
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.44	0.52
2:B:1267:ALA:HB1	2:B:1310:LEU:HD21	1.91	0.52
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.25	0.52
1:A:131:THR:HG21	1:A:143:ARG:HH11	1.75	0.51
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.25	0.51
2:B:1254:VAL:O	2:B:1258:GLN:HG3	2.09	0.51
2:B:1066:LYS:HZ2	2:B:1217:PRO:HB3	1.74	0.51
2:B:1195:ILE:CG2	2:B:1196:GLY:N	2.72	0.51
1:A:178:ILE:CD1	1:A:191:SER:HB3	2.37	0.51
2:B:1278:GLN:O	2:B:1282:LEU:HD13	2.11	0.51
2:B:1247:PRO:O	2:B:1248:GLU:HG3	2.11	0.51
1:A:435:VAL:CG1	2:B:1290:THR:HG21	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1075:VAL:HG11	2:B:1077:PHE:CZ	2.46	0.51
2:B:1160:PHE:CE2	2:B:1164:MET:HE2	2.46	0.51
1:A:412:PRO:HG3	2:B:1401:TRP:CZ2	2.46	0.51
1:A:547:GLN:NE2	1:A:547:GLN:C	2.69	0.51
2:B:1296:THR:HG22	2:B:1297:GLU:N	2.26	0.51
1:A:221:HIS:C	1:A:223:LYS:H	2.19	0.51
1:A:257:ILE:O	1:A:261:VAL:HG23	2.11	0.51
1:A:223:LYS:O	1:A:225:PRO:CD	2.59	0.51
2:B:1266:TRP:C	2:B:1268:SER:H	2.19	0.51
1:A:108:VAL:O	1:A:221:HIS:O	2.28	0.50
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.92	0.50
2:B:1281:LYS:N	2:B:1284:ARG:HE	2.09	0.50
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.93	0.50
2:B:1153:TRP:CZ2	2:B:1155:GLY:HA3	2.46	0.50
2:B:1254:VAL:HG23	2:B:1291:GLU:O	2.11	0.50
1:A:236:PRO:HA	3:A:2000:MSD:HC7	1.93	0.50
2:B:1270:ILE:O	2:B:1271:TYR:HB2	2.11	0.50
2:B:1425:LEU:HB2	2:B:1427:TYR:CE2	2.47	0.50
1:A:388:LYS:HD2	1:A:413:GLU:OE1	2.10	0.50
1:A:297:GLU:O	1:A:301:LEU:HD22	2.12	0.50
2:B:1032:LYS:O	2:B:1035:VAL:HG22	2.12	0.50
1:A:515:SER:HB3	1:A:518:VAL:HB	1.93	0.50
2:B:1255:ASN:O	2:B:1259:LYS:HG3	2.12	0.50
2:B:1280:CYS:C	2:B:1282:LEU:N	2.69	0.50
2:B:1154:LYS:CG	2:B:1184:MET:HE2	2.40	0.50
1:A:238:LYS:HE2	1:A:315:HIS:CD2	2.47	0.49
2:B:1157:PRO:HG2	2:B:1184:MET:HA	1.93	0.49
2:B:1101:LYS:NZ	2:B:1101:LYS:HB3	2.27	0.49
1:A:517:LEU:O	1:A:520:GLN:N	2.45	0.49
1:A:458:VAL:HG11	1:A:547:GLN:NE2	2.28	0.49
1:A:346:PHE:N	1:A:346:PHE:CD2	2.76	0.49
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.48	0.49
1:A:93:GLY:HA3	2:B:1137:ASN:ND2	2.26	0.49
1:A:123:ASP:OD2	1:A:123:ASP:N	2.44	0.49
2:B:1263:LYS:HE2	2:B:1425:LEU:HA	1.94	0.49
2:B:1280:CYS:C	2:B:1284:ARG:HH21	2.20	0.49
2:B:1371:ALA:O	2:B:1375:ILE:HG13	2.13	0.49
2:B:1264:LEU:HB3	2:B:1276:VAL:CG1	2.42	0.49
1:A:350:LYS:HG2	1:A:351:THR:N	2.28	0.49
2:B:1053:GLU:OE1	2:B:1053:GLU:N	2.33	0.49
1:A:194:GLU:O	1:A:198:HIS:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:N	2:B:1284:ARG:HD2	2.27	0.49
1:A:79:GLU:O	1:A:83:ARG:HD2	2.13	0.48
1:A:183:TYR:CE2	1:A:184:MET:HE2	2.48	0.48
1:A:254:VAL:HG21	1:A:288:ALA:O	2.12	0.48
1:A:357:MET:HG3	1:A:358:ARG:N	2.26	0.48
2:B:1154:LYS:O	2:B:1157:PRO:HD2	2.13	0.48
2:B:1283:LEU:HD22	2:B:1293:ILE:CG1	2.43	0.48
2:B:1324:ASP:O	2:B:1343:GLN:HG2	2.12	0.48
1:A:206:ARG:CZ	1:A:217:PRO:O	2.60	0.48
1:A:417:VAL:O	1:A:417:VAL:HG13	2.13	0.48
1:A:77:PHE:O	1:A:78:ARG:C	2.55	0.48
1:A:410:TRP:CG	1:A:411:ILE:N	2.80	0.48
2:B:1066:LYS:NZ	2:B:1217:PRO:HB3	2.28	0.48
1:A:195:ILE:HG23	1:A:199:ARG:CZ	2.44	0.48
2:B:1195:ILE:HD11	2:B:1233:GLU:OE1	2.13	0.48
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.49	0.48
1:A:536:VAL:HG11	2:B:1258:GLN:OE1	2.13	0.48
2:B:1281:LYS:CA	2:B:1284:ARG:HE	2.26	0.48
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.96	0.48
1:A:115:TYR:O	1:A:149:LEU:HB2	2.14	0.48
2:B:1154:LYS:HE3	2:B:1184:MET:CE	2.43	0.48
2:B:1242:GLN:OE1	2:B:1353:LYS:NZ	2.47	0.48
2:B:1303:LEU:O	2:B:1307:ARG:HG2	2.13	0.48
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.43	0.47
2:B:1252:TRP:HB3	2:B:1293:ILE:CD1	2.43	0.47
1:A:221:HIS:O	1:A:222:GLN:HB3	2.14	0.47
2:B:1215:THR:CG2	2:B:1216:THR:H	2.07	0.47
1:A:93:GLY:C	1:A:94:ILE:HD13	2.39	0.47
2:B:1395:LYS:HG2	2:B:1399:GLU:OE1	2.15	0.47
2:B:1422:LEU:HD23	2:B:1422:LEU:C	2.39	0.47
1:A:23:GLN:HG2	1:A:133:PRO:HG3	1.96	0.47
1:A:497:THR:O	1:A:535:TRP:HA	2.15	0.47
2:B:1305:GLU:O	2:B:1308:GLU:HB3	2.14	0.47
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.50	0.47
2:B:1274:ILE:O	2:B:1276:VAL:HG13	2.14	0.47
2:B:1393:ILE:CG1	2:B:1394:GLN:N	2.78	0.47
1:A:37:ILE:HG22	1:A:41:MET:CE	2.44	0.47
1:A:219:LYS:CD	1:A:219:LYS:H	2.26	0.47
2:B:1139:THR:HG22	2:B:1141:GLY:N	2.28	0.47
2:B:1168:LEU:HD13	2:B:1180:ILE:HG21	1.96	0.47
2:B:1216:THR:HB	2:B:1217:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HG3	1:A:72:ARG:NH1	2.30	0.47
1:A:228:LEU:HD13	1:A:242:GLN:OE1	2.15	0.47
1:A:460:ASN:HA	2:B:1286:THR:HG22	1.96	0.47
1:A:519:ASN:O	1:A:523:GLU:HG3	2.14	0.47
1:A:223:LYS:O	1:A:225:PRO:HD3	2.15	0.46
1:A:542:ILE:HG22	1:A:543:GLY:N	2.30	0.46
2:B:1368:LEU:O	2:B:1372:VAL:HG23	2.15	0.46
1:A:126:LYS:NZ	1:A:126:LYS:HB3	2.30	0.46
1:A:209:LEU:HD22	1:A:214:LEU:HD12	1.98	0.46
2:B:1296:THR:HB	2:B:1299:ALA:HB2	1.97	0.46
1:A:238:LYS:HD2	1:A:315:HIS:HB3	1.96	0.46
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.15	0.46
2:B:1090:VAL:HG23	2:B:1091:GLN:H	1.79	0.46
1:A:223:LYS:O	1:A:225:PRO:N	2.49	0.46
1:A:161:GLN:OE1	1:A:182:GLN:NE2	2.48	0.46
1:A:173:LYS:HD3	1:A:173:LYS:C	2.40	0.46
2:B:1137:ASN:C	2:B:1139:THR:H	2.24	0.46
2:B:1139:THR:HG23	2:B:1140:PRO:CD	2.44	0.46
1:A:110:ASP:O	1:A:110:ASP:CG	2.59	0.46
1:A:219:LYS:HD2	1:A:220:LYS:H	1.81	0.46
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.46	0.46
2:B:1379:SER:OG	2:B:1387:PRO:HD3	2.15	0.46
1:A:487:GLN:O	1:A:489:SER:N	2.46	0.46
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.51	0.46
2:B:1154:LYS:HE3	2:B:1184:MET:HE1	1.98	0.46
2:B:1231:GLY:O	2:B:1232:TYR:CB	2.64	0.46
2:B:1139:THR:HG22	2:B:1141:GLY:H	1.81	0.46
2:B:1266:TRP:CE3	2:B:1425:LEU:HD21	2.51	0.46
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.99	0.45
1:A:222:GLN:O	1:A:223:LYS:C	2.58	0.45
2:B:1051:GLY:HA3	2:B:1053:GLU:OE1	2.16	0.45
2:B:1296:THR:CG2	2:B:1297:GLU:N	2.79	0.45
2:B:1395:LYS:O	2:B:1399:GLU:HG3	2.16	0.45
1:A:124:PHE:O	1:A:127:TYR:HD2	1.98	0.45
1:A:365:VAL:HG21	1:A:425:LEU:HD21	1.98	0.45
2:B:1414:TRP:HD1	2:B:1414:TRP:O	1.99	0.45
1:A:100:LEU:HD21	3:A:2000:MSD:H443	1.99	0.45
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.52	0.45
2:B:1077:PHE:O	2:B:1078:ARG:C	2.58	0.45
1:A:406:TRP:CH2	2:B:1418:ASN:HA	2.52	0.45
2:B:1296:THR:HB	2:B:1299:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1267:ALA:O	2:B:1274:ILE:HG13	2.16	0.45
2:B:1195:ILE:CG2	2:B:1196:GLY:H	2.29	0.45
2:B:1257:ILE:O	2:B:1257:ILE:HD12	2.16	0.45
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.17	0.45
2:B:1414:TRP:O	2:B:1414:TRP:CD1	2.70	0.45
2:B:1417:VAL:HG22	2:B:1418:ASN:N	2.28	0.45
1:A:275:LYS:HG2	1:A:336:GLN:NE2	2.31	0.45
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.52	0.45
1:A:522:ILE:O	1:A:526:ILE:HG13	2.17	0.45
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.82	0.45
2:B:1100:LEU:HG	2:B:1381:VAL:HG13	1.97	0.45
2:B:1252:TRP:HB3	2:B:1293:ILE:HD13	1.98	0.45
2:B:1365:VAL:O	2:B:1369:THR:HG23	2.17	0.45
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.82	0.44
2:B:1079:GLU:HB2	4:B:3007:HOH:O	2.17	0.44
1:A:210:LEU:C	1:A:212:TRP:H	2.25	0.44
2:B:1266:TRP:CE2	2:B:1425:LEU:HD11	2.52	0.44
1:A:194:GLU:C	1:A:196:GLY:N	2.75	0.44
1:A:362:THR:O	1:A:512:LYS:HG2	2.18	0.44
2:B:1085:GLN:HA	2:B:1088:TRP:NE1	2.33	0.44
2:B:1084:THR:O	2:B:1085:GLN:C	2.61	0.44
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.53	0.44
2:B:1031:ILE:O	2:B:1035:VAL:HG13	2.17	0.44
2:B:1420:PRO:O	2:B:1422:LEU:N	2.48	0.44
2:B:1279:LEU:N	2:B:1302:GLU:OE1	2.50	0.44
1:A:344:GLU:HG2	1:A:347:LYS:HD3	1.99	0.44
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.17	0.43
1:A:494:ASN:HB3	2:B:1289:LEU:HD12	1.99	0.43
2:B:1294:PRO:O	2:B:1295:LEU:HD23	2.18	0.43
1:A:31:ILE:O	1:A:35:VAL:HG23	2.18	0.43
1:A:409:THR:O	2:B:1364:ASP:HB2	2.17	0.43
1:A:351:THR:CG2	1:A:352:GLY:N	2.81	0.43
1:A:361:HIS:HD2	1:A:513:SER:OG	2.00	0.43
1:A:450:THR:HG22	1:A:452:LEU:HG	1.99	0.43
1:A:16:MET:HE2	1:A:83:ARG:CG	2.48	0.43
1:A:410:TRP:HA	1:A:410:TRP:HE3	1.82	0.43
2:B:1326:ILE:O	2:B:1341:ILE:HA	2.18	0.43
1:A:183:TYR:CZ	1:A:184:MET:HE2	2.54	0.43
2:B:1063:ILE:CD1	2:B:1074:LEU:HD22	2.44	0.43
2:B:1073:LYS:NZ	2:B:1130:PHE:CZ	2.84	0.43
2:B:1214:LEU:HD12	2:B:1214:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:CG	1:A:66:LYS:H	2.21	0.43
2:B:1103:ASN:OD1	2:B:1179:VAL:HG21	2.18	0.43
2:B:1344:GLU:O	2:B:1345:PRO:C	2.62	0.43
2:B:1353:LYS:NZ	2:B:1353:LYS:HB3	2.34	0.43
1:A:56:TYR:O	1:A:129:ALA:HB3	2.19	0.42
1:A:131:THR:HG23	1:A:143:ARG:NH1	2.34	0.42
1:A:252:TRP:HB3	1:A:257:ILE:CD1	2.48	0.42
1:A:273:GLY:HA2	1:A:332:GLN:OE1	2.19	0.42
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.01	0.42
1:A:548:VAL:O	1:A:552:VAL:HG23	2.20	0.42
1:A:428:GLN:HA	1:A:509:GLN:HE21	1.84	0.42
1:A:447:ASN:HB3	1:A:450:THR:HB	2.00	0.42
2:B:1426:TRP:HA	2:B:1426:TRP:CE3	2.53	0.42
2:B:1028:GLU:HG2	2:B:1032:LYS:HE2	2.00	0.42
2:B:1420:PRO:C	2:B:1422:LEU:N	2.69	0.42
1:A:26:LEU:O	1:A:31:ILE:HD11	2.20	0.42
1:A:406:TRP:CD2	1:A:407:GLN:N	2.88	0.42
1:A:406:TRP:CE3	2:B:1419:THR:HB	2.54	0.42
2:B:1282:LEU:CB	2:B:1283:LEU:HD12	2.46	0.42
1:A:107:THR:HA	1:A:223:LYS:CB	2.49	0.42
1:A:218:ASP:OD1	1:A:219:LYS:HE2	2.20	0.42
1:A:396:GLU:O	1:A:397:THR:C	2.62	0.42
2:B:1039:THR:HG23	2:B:1043:LYS:NZ	2.34	0.42
2:B:1296:THR:HG22	2:B:1299:ALA:H	1.85	0.42
1:A:553:SER:O	1:A:555:GLY:N	2.53	0.42
2:B:1264:LEU:HB3	2:B:1276:VAL:HG11	2.01	0.42
1:A:171:PHE:CD1	1:A:171:PHE:C	2.97	0.42
1:A:517:LEU:HD22	1:A:521:ILE:HD11	2.01	0.42
2:B:1067:ASP:OD2	2:B:1407:GLN:NE2	2.53	0.42
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.50	0.42
1:A:234:LEU:N	1:A:234:LEU:CD1	2.82	0.42
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.01	0.42
2:B:1252:TRP:O	2:B:1292:VAL:HG23	2.20	0.42
2:B:1280:CYS:SG	2:B:1281:LYS:N	2.92	0.42
2:B:1330:GLN:NE2	2:B:1338:THR:OG1	2.52	0.42
1:A:94:ILE:O	1:A:95:PRO:C	2.60	0.42
1:A:451:LYS:HB3	1:A:471:ASN:HA	2.02	0.42
2:B:1079:GLU:O	2:B:1082:LYS:HB2	2.20	0.42
1:A:195:ILE:HG23	1:A:199:ARG:HD2	2.02	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.77	0.41
1:A:317:VAL:HG22	1:A:318:TYR:H	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:C	1:A:551:LEU:HD12	2.45	0.41
2:B:1266:TRP:CG	2:B:1427:TYR:HH	2.32	0.41
1:A:21:VAL:HB	1:A:59:PRO:CD	2.48	0.41
1:A:40:GLU:O	1:A:44:GLU:HG3	2.21	0.41
2:B:1028:GLU:CG	2:B:1032:LYS:HE2	2.51	0.41
2:B:1254:VAL:HG21	2:B:1288:ALA:O	2.20	0.41
1:A:223:LYS:O	1:A:224:GLU:C	2.63	0.41
1:A:420:PRO:HA	1:A:421:PRO:O	2.20	0.41
2:B:1077:PHE:HD2	2:B:1152:GLY:CA	2.32	0.41
2:B:1293:ILE:HD13	2:B:1293:ILE:H	1.86	0.41
1:A:111:VAL:HG21	1:A:164:MET:CE	2.49	0.41
1:A:271:TYR:O	1:A:274:ILE:HG12	2.20	0.41
1:A:395:LYS:O	1:A:399:GLU:HB2	2.19	0.41
1:A:410:TRP:CG	1:A:411:ILE:H	2.38	0.41
2:B:1051:GLY:C	2:B:1053:GLU:OE1	2.64	0.41
1:A:241:VAL:O	1:A:242:GLN:C	2.64	0.41
1:A:555:GLY:O	1:A:556:ILE:C	2.63	0.41
1:A:65:LYS:HZ3	1:A:72:ARG:HD2	1.85	0.41
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.55	0.41
1:A:24:TRP:O	1:A:26:LEU:HD22	2.21	0.41
1:A:105:SER:HB3	1:A:198:HIS:CD2	2.56	0.41
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.01	0.41
2:B:1073:LYS:HE2	2:B:1075:VAL:HG23	2.02	0.41
2:B:1207:GLN:O	2:B:1211:ARG:HD3	2.21	0.41
2:B:1419:THR:HG22	2:B:1420:PRO:O	2.21	0.41
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.55	0.41
1:A:366:LYS:O	1:A:370:GLU:HG3	2.21	0.41
1:A:317:VAL:CG2	1:A:318:TYR:N	2.84	0.40
2:B:1264:LEU:HB3	2:B:1276:VAL:HG12	2.03	0.40
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.55	0.40
1:A:216:THR:OG1	1:A:217:PRO:HD2	2.21	0.40
2:B:1091:GLN:C	2:B:1092:LEU:HD23	2.46	0.40
2:B:1125:ARG:HD3	2:B:1147:ASN:HA	2.02	0.40
2:B:1163:SER:O	2:B:1167:ILE:HG13	2.21	0.40
1:A:100:LEU:CD2	3:A:2000:MSD:H443	2.51	0.40
1:A:305:GLU:O	1:A:308:GLU:HB3	2.22	0.40
1:A:369:THR:HG22	1:A:370:GLU:N	2.37	0.40
2:B:1271:TYR:CD2	2:B:1310:LEU:HA	2.56	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.93	0.40
1:A:206:ARG:HE	1:A:216:THR:CG2	2.30	0.40
2:B:1193:LEU:CD1	2:B:1193:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1241:VAL:HG12	2:B:1242:GLN:N	2.34	0.40
2:B:1393:ILE:CG1	2:B:1394:GLN:H	2.34	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:NH2	1:A:448:ARG:NH2[3_557]	1.64	0.56

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	555/560 (99%)	475 (86%)	60 (11%)	20 (4%)	2	16
2	B	399/427 (93%)	342 (86%)	46 (12%)	11 (3%)	4	21
All	All	954/987 (97%)	817 (86%)	106 (11%)	31 (3%)	3	18

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
2	B	1065	LYS
2	B	1085	GLN
2	B	1294	PRO
1	A	18	GLY
1	A	137	ASN
1	A	224	GLU
1	A	430	GLU
1	A	554	ALA
2	B	1267	ALA
1	A	114	ALA

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Mol	Chain	Res	Type
1	A	247	PRO
1	A	332	GLN
1	A	333	GLY
1	A	345	PRO
1	A	412	PRO
2	B	1184	MET
2	B	1215	THR
2	B	1232	TYR
2	B	1286	THR
1	A	226	PRO
1	A	487	GLN
2	B	1185	ASP
1	A	151	GLN
1	A	358	ARG
1	A	427	TYR
2	B	1213	GLY
1	A	230	MET
1	A	217	PRO
2	B	1111	VAL
1	A	381	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/500 (99%)	452 (91%)	43 (9%)	9	35
2	B	369/389 (95%)	342 (93%)	27 (7%)	13	42
All	All	864/889 (97%)	794 (92%)	70 (8%)	11	38

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	14	PRO
1	A	21	VAL

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	101	LYS
1	A	110	ASP
1	A	123	ASP
1	A	126	LYS
1	A	139	THR
1	A	151	GLN
1	A	159	ILE
1	A	174	GLN
1	A	182	GLN
1	A	187	LEU
1	A	195	ILE
1	A	210	LEU
1	A	215	THR
1	A	219	LYS
1	A	226	PRO
1	A	227	PHE
1	A	228	LEU
1	A	245	VAL
1	A	247	PRO
1	A	259	LYS
1	A	260	LEU
1	A	280	CYS
1	A	297	GLU
1	A	301	LEU
1	A	325	LEU
1	A	338	THR
1	A	344	GLU
1	A	345	PRO
1	A	349	LEU
1	A	361	HIS
1	A	369	THR
1	A	402	TRP
1	A	424	LYS
1	A	432	GLU
1	A	459	THR
1	A	488	ASP
1	A	517	LEU
1	A	531	VAL
1	A	547	GLN
2	B	1010	VAL
2	B	1039	THR

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Mol	Chain	Res	Type
2	B	1058	THR
2	B	1078	ARG
2	B	1101	LYS
2	B	1122	GLU
2	B	1138	GLU
2	B	1139	THR
2	B	1185	ASP
2	B	1201	LYS
2	B	1241	VAL
2	B	1250	ASP
2	B	1252	TRP
2	B	1257	ILE
2	B	1260	LEU
2	B	1283	LEU
2	B	1292	VAL
2	B	1293	ILE
2	B	1297	GLU
2	B	1330	GLN
2	B	1353	LYS
2	B	1363	ASN
2	B	1366	LYS
2	B	1370	GLU
2	B	1422	LEU
2	B	1425	LEU
2	B	1426	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	136	ASN
1	A	145	GLN
1	A	151	GLN
1	A	221	HIS
1	A	315	HIS
1	A	332	GLN
1	A	336	GLN
1	A	361	HIS
1	A	407	GLN
1	A	475	GLN
1	A	509	GLN
1	A	524	GLN

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Mol	Chain	Res	Type
1	A	539	HIS
1	A	547	GLN
2	B	1137	ASN
2	B	1161	GLN
2	B	1182	GLN
2	B	1255	ASN
2	B	1306	ASN
2	B	1332	GLN
2	B	1394	GLN
2	B	1407	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 ⓘ

1 ligand is 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$
3	MSD	A	2000	-	28,29,29	4.30	19 (67%)	33,41,41	2.34	14 (42%)

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
3	MSD	A	2000	-	-	4/20/25/25	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	MSD	C9-S10	-16.66	1.29	1.68
3	A	2000	MSD	O41-C44	-5.95	1.26	1.42
3	A	2000	MSD	C21-C15	5.37	1.49	1.40
3	A	2000	MSD	C13-C14	4.75	1.58	1.50
3	A	2000	MSD	C5-N4	3.92	1.41	1.34
3	A	2000	MSD	C20-C21	3.65	1.47	1.41
3	A	2000	MSD	C2-C42	3.61	1.52	1.44
3	A	2000	MSD	C7-C2	3.40	1.46	1.39
3	A	2000	MSD	C7-C6	3.23	1.44	1.38
3	A	2000	MSD	C13-C12	3.21	1.53	1.49
3	A	2000	MSD	C18-C16	3.00	1.45	1.39
3	A	2000	MSD	C19-C20	2.98	1.44	1.39
3	A	2000	MSD	C15-C14	2.86	1.56	1.52
3	A	2000	MSD	C3-C2	2.77	1.43	1.39
3	A	2000	MSD	C20-C23	2.73	1.54	1.48
3	A	2000	MSD	C19-C18	2.62	1.43	1.38
3	A	2000	MSD	C3-N4	2.53	1.39	1.34
3	A	2000	MSD	C9-N11	2.39	1.38	1.34
3	A	2000	MSD	C16-C15	2.34	1.43	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	MSD	C3-N4-C5	6.34	123.78	117.83
3	A	2000	MSD	C44-O41-C16	4.99	124.84	117.51
3	A	2000	MSD	C3-C2-C42	4.30	124.63	120.05
3	A	2000	MSD	C5-N8-C9	-3.86	126.59	130.74
3	A	2000	MSD	O41-C16-C15	3.48	119.15	115.51
3	A	2000	MSD	C2-C3-N4	-3.34	118.72	123.50
3	A	2000	MSD	C13-C14-C15	-3.25	116.03	122.24
3	A	2000	MSD	C12-N11-C9	-2.63	121.22	125.61
3	A	2000	MSD	C16-C15-C14	-2.29	115.65	122.11
3	A	2000	MSD	C2-C42-N43	-2.16	172.53	177.87
3	A	2000	MSD	C25-C23-C20	2.10	123.11	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	MSD	O41-C16-C18	-2.05	120.84	124.30
3	A	2000	MSD	C7-C2-C42	-2.05	116.64	119.97
3	A	2000	MSD	C6-C5-N4	-2.02	119.54	122.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

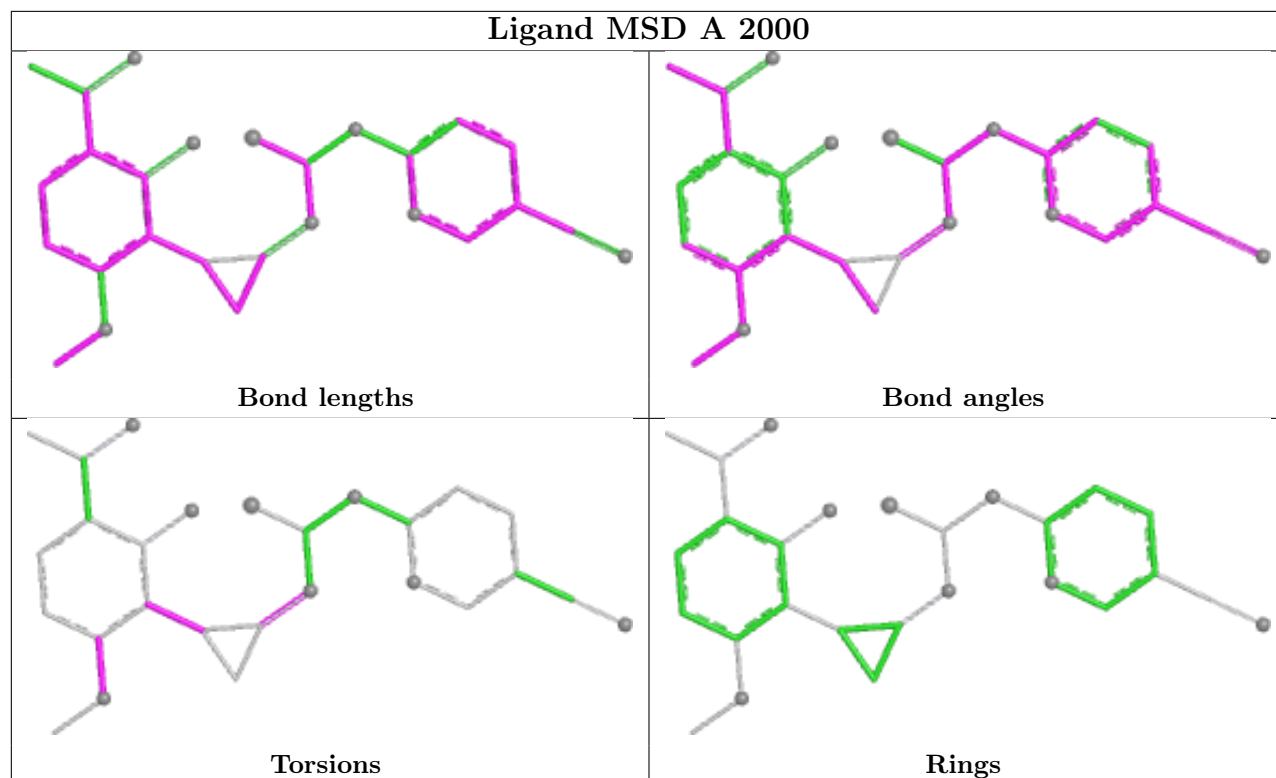
Mol	Chain	Res	Type	Atoms
3	A	2000	MSD	C14-C12-N11-C9
3	A	2000	MSD	C13-C14-C15-C21
3	A	2000	MSD	C18-C16-O41-C44
3	A	2000	MSD	C15-C16-O41-C44

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	MSD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	557/560 (99%)	-0.22	2 (0%)	88 76	20, 56, 91, 130	2 (0%)
2	B	405/427 (94%)	-0.20	13 (3%)	50 29	19, 49, 109, 133	9 (2%)
All	All	962/987 (97%)	-0.21	15 (1%)	70 47	19, 53, 104, 133	11 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1217	PRO	3.5
2	B	1427	TYR	3.1
2	B	1005	ILE	3.1
2	B	1363	ASN	2.9
2	B	1253	THR	2.8
2	B	1426	TRP	2.6
2	B	1362	THR	2.6
1	A	547	GLN	2.4
2	B	1231	GLY	2.4
1	A	223	LYS	2.4
2	B	1421	PRO	2.1
2	B	1425	LEU	2.1
2	B	1267	ALA	2.1
2	B	1424	LYS	2.0
2	B	1283	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

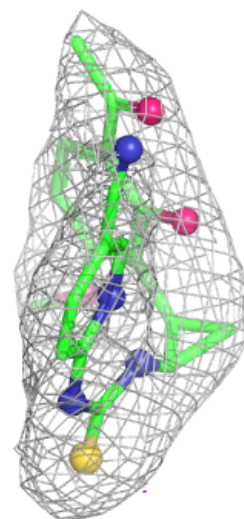
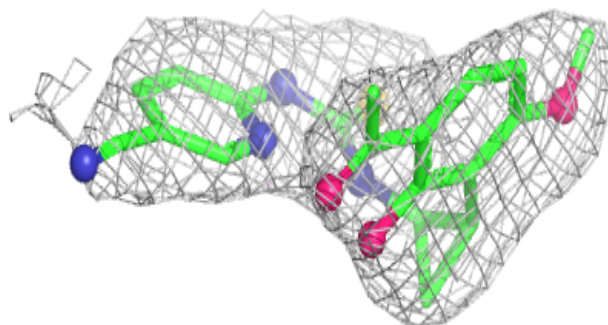
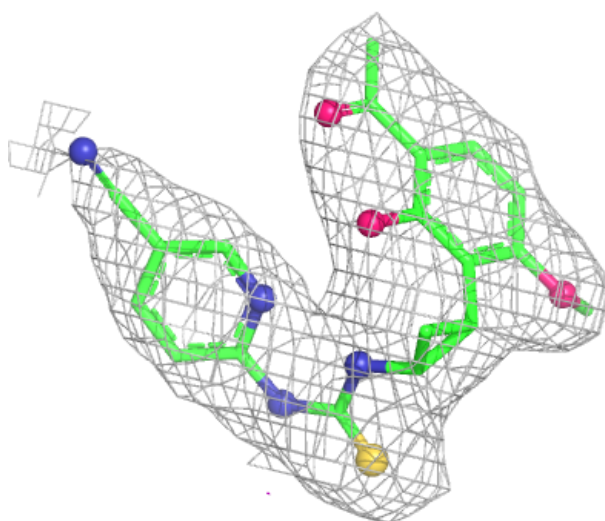
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MSD	A	2000	27/27	0.96	0.08	28,34,39,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MSD A 2000:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.