



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 1FKP / pdb_00001fkp
Title : CRYSTAL STRUCTURE OF NNRTI RESISTANT K103N MUTANT HIV-1
REVERSE TRANSCRIPTASE IN COMPLEX WITH NEVIRAPINE
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Deposited on : 2000-08-10
Resolution : 2.90 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

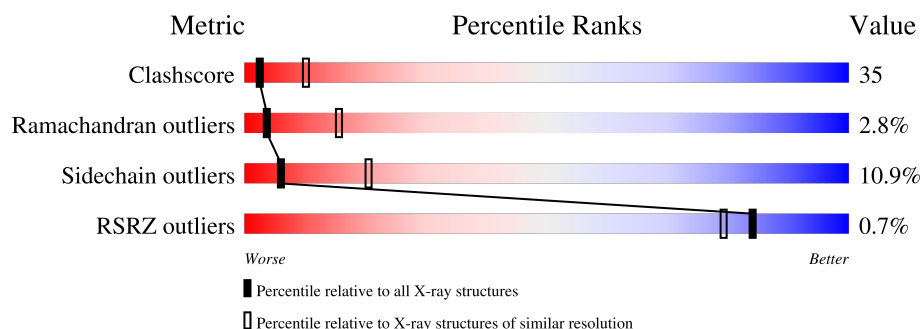
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	543	35% 52% 11% .
2	B	440	39% 44% 9% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7814 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 HIV-1 RT, A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4430	2865	738	819	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LEU	engineered mutation	UNP P04585

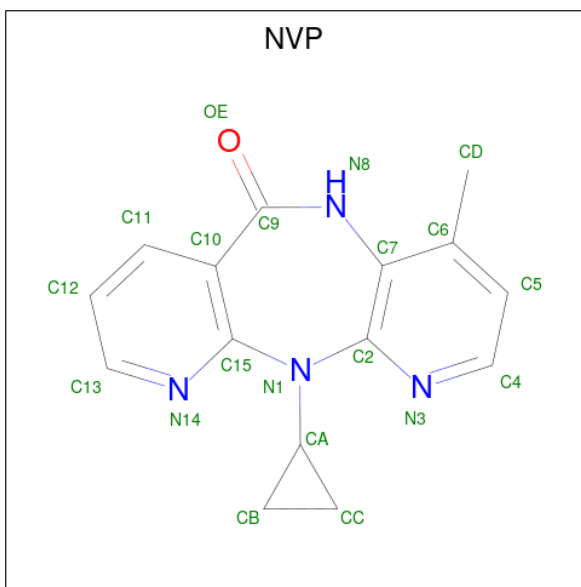
- Molecule 2 is a protein called HIV-1 RT, B-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total	C	N	O	S	0	0	0
			3364	2183	560	614	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LEU	engineered mutation	UNP P04585

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (CCD ID: NVP) (formula: C₁₅H₁₄N₄O).

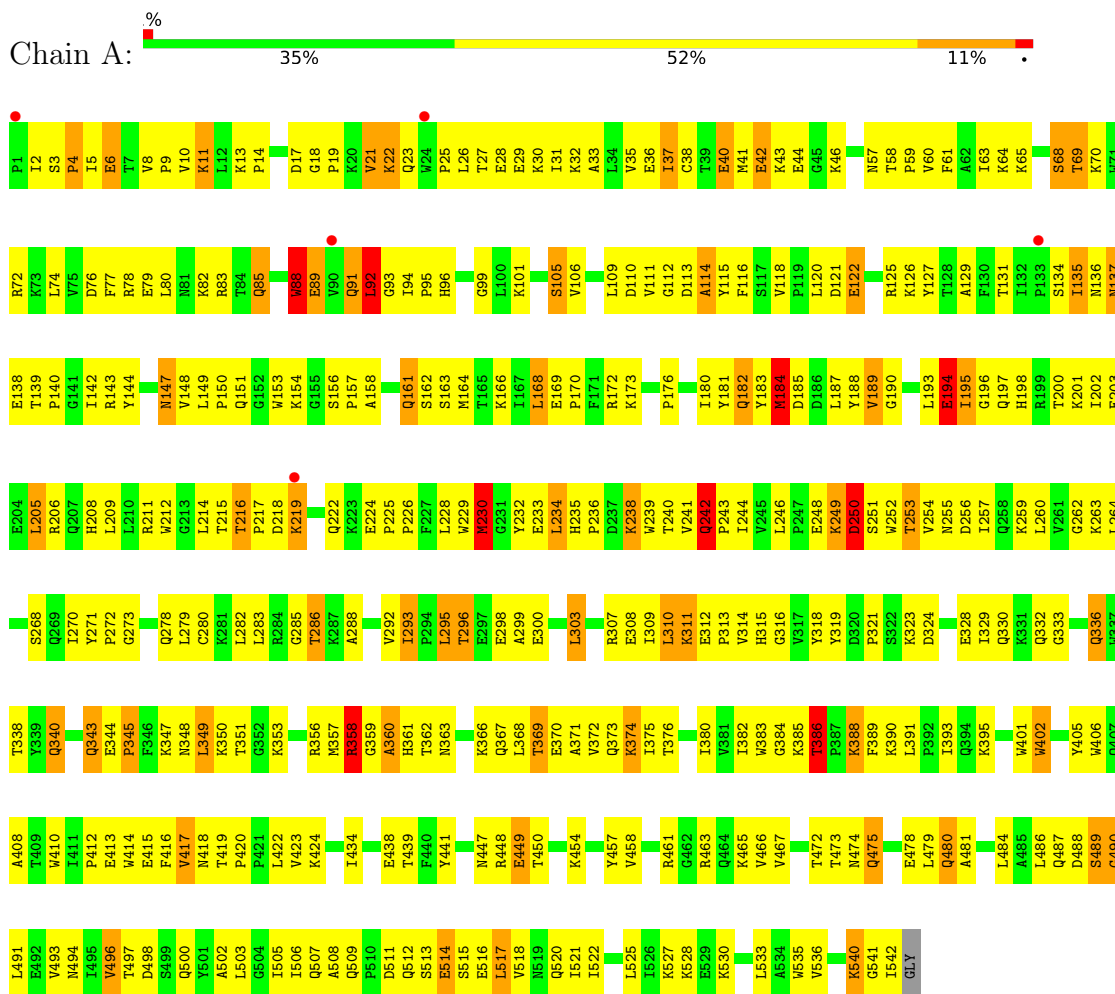


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	20	15	4	1	0	0

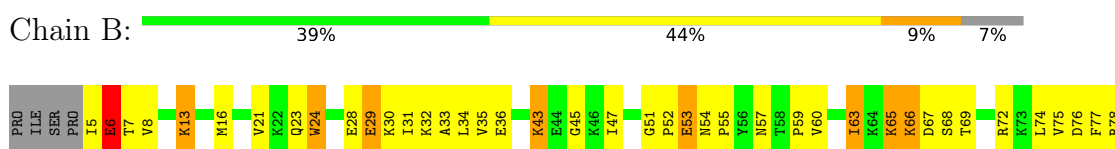
3 Residue-property plots

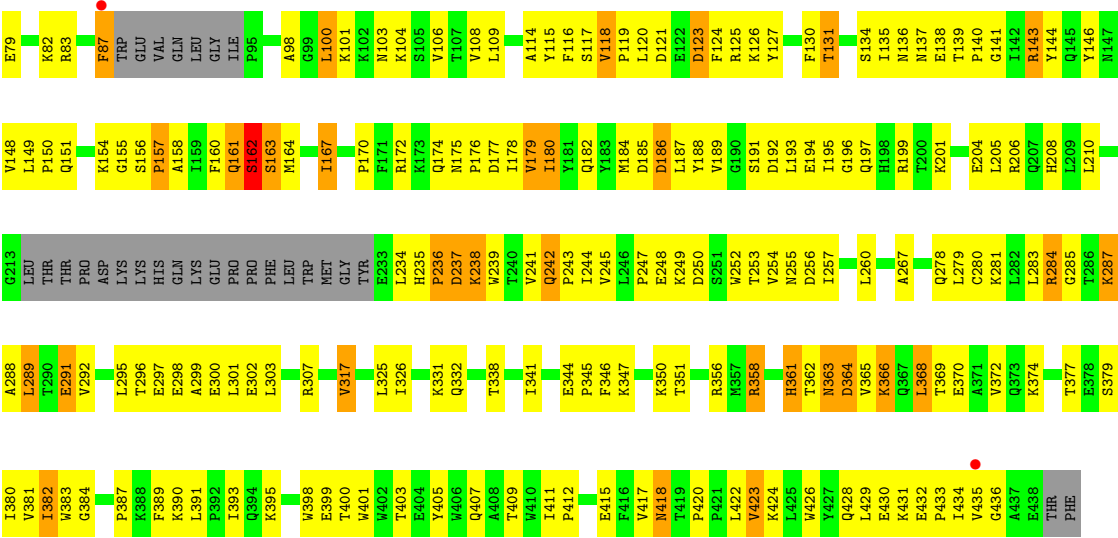
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: HIV-1 RT, A-CHAIN



• Molecule 2: HIV-1 RT, B-CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.70Å 109.80Å 72.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.90) 93.0 (30.00-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.281 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7814	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: CSD, NVP

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	0.61	0/4539	1.10	31/6170 (0.5%)
2	B	0.58	0/3456	1.11	24/4692 (0.5%)
All	All	0.60	0/7995	1.11	55/10862 (0.5%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	LYS	N-CA-C	8.81	123.42	109.50
2	B	417	VAL	N-CA-C	8.76	119.51	108.82
1	A	271	TYR	CA-C-N	-8.66	110.65	119.92
1	A	271	TYR	C-N-CA	-8.66	110.65	119.92
2	B	382	ILE	N-CA-C	8.51	119.07	110.82
2	B	118	VAL	N-CA-C	8.50	117.28	108.95
1	A	388	LYS	N-CA-C	-8.35	97.00	110.20
2	B	13	LYS	N-CA-C	-8.10	99.36	109.64
1	A	489	SER	N-CA-C	8.03	123.60	112.04
1	A	386	THR	CA-C-N	7.88	127.81	119.85
1	A	386	THR	C-N-CA	7.88	127.81	119.85
1	A	114	ALA	N-CA-C	-7.43	103.67	112.89
2	B	131	THR	N-CA-C	7.41	120.56	108.26
1	A	273	GLY	N-CA-C	-7.25	105.31	113.79
2	B	66	LYS	N-CA-C	-7.13	100.65	110.35
2	B	156	SER	CA-C-N	-6.87	112.63	119.56
2	B	156	SER	C-N-CA	-6.87	112.63	119.56
1	A	402	TRP	N-CA-C	6.76	118.73	111.36
1	A	147	ASN	N-CA-C	-6.75	104.26	113.30
2	B	422	LEU	N-CA-C	6.63	118.30	111.14
1	A	343	GLN	N-CA-C	-6.62	105.09	113.43
1	A	234	LEU	N-CA-C	6.61	119.71	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	ASP	N-CA-C	-6.57	103.61	111.69
1	A	401	TRP	N-CA-C	6.54	118.20	111.14
2	B	391	LEU	N-CA-C	6.52	119.08	109.62
2	B	6	GLU	N-CA-C	-6.46	100.28	109.96
2	B	235	HIS	CA-C-N	6.42	127.87	119.84
2	B	235	HIS	C-N-CA	6.42	127.87	119.84
2	B	428	GLN	N-CA-C	-6.33	103.64	111.75
1	A	311	LYS	N-CA-C	-6.25	103.14	111.96
1	A	314	VAL	N-CA-C	6.21	116.80	108.11
1	A	293	ILE	N-CA-C	6.14	114.58	107.89
1	A	391	LEU	N-CA-C	6.13	119.39	110.14
1	A	490	GLY	N-CA-C	-6.10	105.82	112.04
1	A	503	LEU	N-CA-C	-6.01	104.81	111.36
2	B	157	PRO	N-CA-C	-5.92	106.47	113.86
1	A	348	ASN	N-CA-C	5.91	118.82	109.96
1	A	184	MET	CB-CA-C	-5.88	109.23	117.23
1	A	131	THR	N-CA-C	5.67	118.72	109.24
2	B	53	GLU	N-CA-C	-5.62	104.55	111.75
1	A	494	ASN	N-CA-C	-5.60	99.77	108.90
2	B	400	THR	N-CA-C	5.56	118.11	111.71
2	B	364	ASP	N-CA-C	5.54	117.00	111.07
2	B	317	VAL	N-CA-C	5.50	115.24	106.88
1	A	389	PHE	N-CA-C	5.48	118.66	109.95
1	A	242	GLN	CA-C-N	5.36	139.87	127.00
1	A	242	GLN	C-N-CA	5.36	139.87	127.00
1	A	458	VAL	N-CA-C	-5.35	101.21	108.06
2	B	143	ARG	N-CA-C	5.26	117.31	109.25
1	A	507	GLN	N-CA-C	5.25	117.09	111.36
2	B	326	ILE	N-CA-C	5.22	116.10	108.53
2	B	156	SER	N-CA-C	5.19	119.81	112.75
1	A	417	VAL	N-CA-C	-5.19	100.85	108.11
1	A	194	GLU	N-CA-C	-5.14	103.25	110.50
2	B	43	LYS	N-CA-C	-5.01	105.71	111.07

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	4430	0	4474	347	0
2	B	3364	0	3393	213	0
3	A	20	0	14	2	0
All	All	7814	0	7881	542	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 35.

All (542) 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:239:TRP:CZ2	1:A:316:GLY:HA3	2.00	0.96
1:A:65:LYS:HB3	1:A:72:ARG:HD3	1.46	0.96
1:A:358:ARG:NH1	1:A:358:ARG:HB3	1.81	0.96
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.46	0.93
2:B:395:LYS:O	2:B:399:GLU:HG2	1.70	0.92
1:A:23:GLN:HE22	1:A:60:VAL:H	1.05	0.90
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.05	0.90
1:A:138:GLU:HG3	1:A:139:THR:H	1.37	0.88
1:A:61:PHE:HB2	1:A:74:LEU:HD21	1.55	0.88
2:B:356:ARG:NH2	2:B:361:HIS:ND1	2.22	0.88
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.56	0.87
2:B:242:GLN:HA	2:B:242:GLN:HE21	1.38	0.86
1:A:136:ASN:OD1	1:A:138:GLU:HB3	1.80	0.82
1:A:61:PHE:HB2	1:A:74:LEU:CD2	2.09	0.82
1:A:184:MET:HE3	1:A:184:MET:HA	1.59	0.82
1:A:448:ARG:HG3	1:A:449:GLU:HG2	1.59	0.82
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.60	0.81
1:A:161:GLN:HE21	1:A:161:GLN:C	1.89	0.80
2:B:420:PRO:HB2	2:B:423:VAL:HG13	1.63	0.80
1:A:17:ASP:O	1:A:83:ARG:HD3	1.82	0.80
1:A:125:ARG:NH1	1:A:147:ASN:HB3	1.97	0.79
1:A:79:GLU:HG3	1:A:83:ARG:NH1	1.98	0.79
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.66	0.78
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.00	0.77
2:B:157:PRO:HG2	2:B:184:MET:HA	1.66	0.77
1:A:122:GLU:H	1:A:122:GLU:CD	1.90	0.76
1:A:6:GLU:H	1:A:6:GLU:CD	1.94	0.76
2:B:158:ALA:O	2:B:161:GLN:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ALA:O	1:A:506:ILE:HD12	1.87	0.75
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.66	0.75
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.69	0.75
2:B:247:PRO:HB2	2:B:249:LYS:NZ	2.03	0.74
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.73	0.71
1:A:193:LEU:HB3	1:A:197:GLN:HE21	1.55	0.71
2:B:13:LYS:HE2	2:B:82:LYS:O	1.91	0.71
1:A:244:ILE:CG2	1:A:310:LEU:HD13	2.21	0.71
1:A:358:ARG:HB3	1:A:358:ARG:HH11	1.56	0.71
1:A:206:ARG:NH2	1:A:218:ASP:HB3	2.06	0.70
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.74	0.70
2:B:100:LEU:HD23	2:B:100:LEU:H	1.57	0.70
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.07	0.69
2:B:182:GLN:HB2	2:B:187:LEU:HD12	1.74	0.69
1:A:366:LYS:O	1:A:369:THR:HB	1.93	0.69
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.27	0.69
1:A:506:ILE:HG13	1:A:533:LEU:HD23	1.75	0.69
2:B:65:LYS:HZ3	2:B:72:ARG:HD3	1.59	0.68
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.29	0.68
1:A:234:LEU:HD12	1:A:234:LEU:N	2.08	0.68
1:A:270:ILE:O	1:A:272:PRO:HD3	1.94	0.67
2:B:170:PRO:O	2:B:174:GLN:HG2	1.94	0.67
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.29	0.67
2:B:5:ILE:CG1	2:B:6:GLU:N	2.58	0.67
2:B:197:GLN:O	2:B:201:LYS:HB2	1.95	0.67
1:A:497:THR:O	1:A:535:TRP:HA	1.95	0.67
2:B:155:GLY:O	2:B:158:ALA:HB3	1.95	0.67
1:A:235:HIS:ND1	1:A:238:LYS:HE3	2.09	0.67
1:A:31:ILE:O	1:A:35:VAL:HG23	1.95	0.66
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.25	0.66
2:B:16:MET:HE3	2:B:83:ARG:HA	1.78	0.66
2:B:238:LYS:O	2:B:239:TRP:HD1	1.78	0.66
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.77	0.65
1:A:358:ARG:HH22	1:A:512:GLN:HB2	1.60	0.65
1:A:358:ARG:HB3	1:A:358:ARG:CZ	2.25	0.65
1:A:68:SER:C	1:A:70:LYS:H	2.04	0.65
2:B:237:ASP:O	2:B:239:TRP:N	2.28	0.65
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.32	0.65
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.78	0.65
1:A:22:LYS:H	1:A:22:LYS:HD3	1.62	0.64
1:A:184:MET:HA	1:A:184:MET:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.79	0.64
2:B:426:TRP:O	2:B:429:LEU:HB2	1.97	0.64
1:A:229:TRP:O	1:A:230:MET:C	2.41	0.64
2:B:100:LEU:H	2:B:100:LEU:CD2	2.11	0.64
2:B:242:GLN:HA	2:B:242:GLN:NE2	2.13	0.64
1:A:383:TRP:O	1:A:385:LYS:HG2	1.98	0.64
2:B:79:GLU:O	2:B:83:ARG:HG3	1.98	0.64
1:A:242:GLN:HB3	1:A:243:PRO:O	1.98	0.63
2:B:23:GLN:OE1	2:B:59:PRO:HA	1.99	0.63
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.34	0.63
1:A:40:GLU:OE2	1:A:43:LYS:NZ	2.32	0.63
1:A:253:THR:HG23	1:A:256:ASP:OD1	1.99	0.63
2:B:100:LEU:HD23	2:B:100:LEU:N	2.14	0.63
2:B:242:GLN:HB2	2:B:430:GLU:OE1	1.99	0.62
2:B:356:ARG:HH22	2:B:361:HIS:CE1	2.17	0.62
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.34	0.62
2:B:120:LEU:HD21	2:B:124:PHE:HD2	1.64	0.62
1:A:517:LEU:O	1:A:520:GLN:HB2	1.98	0.62
2:B:180:ILE:HD11	2:B:189:VAL:HG13	1.82	0.62
1:A:541:GLY:HA3	2:B:284:ARG:CZ	2.30	0.61
1:A:40:GLU:O	1:A:43:LYS:HG2	2.00	0.61
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.82	0.61
1:A:358:ARG:NH2	1:A:512:GLN:HB2	2.16	0.61
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.35	0.61
2:B:390:LYS:HE2	2:B:415:GLU:OE2	1.99	0.61
2:B:65:LYS:NZ	2:B:72:ARG:HD3	2.14	0.61
2:B:154:LYS:O	2:B:157:PRO:HD2	2.01	0.61
1:A:255:ASN:O	1:A:259:LYS:HG3	2.00	0.61
1:A:22:LYS:H	1:A:22:LYS:CD	2.15	0.60
1:A:489:SER:OG	1:A:528:LYS:NZ	2.28	0.60
1:A:142:ILE:N	1:A:142:ILE:HD12	2.16	0.60
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.26	0.60
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.65	0.60
1:A:235:HIS:HB2	1:A:238:LYS:HD2	1.83	0.60
1:A:382:ILE:O	2:B:135:ILE:HG22	2.00	0.60
1:A:22:LYS:HD3	1:A:22:LYS:N	2.17	0.60
1:A:195:ILE:HG13	1:A:196:GLY:N	2.17	0.60
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.01	0.60
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.84	0.60
1:A:195:ILE:HG13	1:A:196:GLY:H	1.66	0.59
2:B:254:VAL:HB	2:B:289:LEU:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.02	0.59
2:B:278:GLN:HB2	2:B:302:GLU:OE2	2.02	0.59
1:A:490:GLY:H	1:A:528:LYS:NZ	1.99	0.59
2:B:5:ILE:CG1	2:B:6:GLU:H	2.16	0.59
2:B:253:THR:O	2:B:257:ILE:HG12	2.03	0.59
2:B:424:LYS:C	2:B:424:LYS:HD2	2.27	0.59
1:A:540:LYS:HG2	2:B:280:CYS:SG	2.42	0.59
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.02	0.59
1:A:257:ILE:O	1:A:260:LEU:HB3	2.02	0.58
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.32	0.58
2:B:5:ILE:HG12	2:B:6:GLU:N	2.17	0.58
1:A:38:CYS:O	1:A:42:GLU:HB2	2.04	0.58
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.18	0.58
2:B:135:ILE:O	2:B:138:GLU:HG2	2.03	0.58
2:B:247:PRO:HB2	2:B:249:LYS:HZ2	1.68	0.58
2:B:5:ILE:HG13	2:B:6:GLU:H	1.67	0.58
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.83	0.58
1:A:243:PRO:HG3	1:A:313:PRO:HA	1.85	0.58
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.58
1:A:42:GLU:CG	1:A:144:TYR:HE2	2.17	0.57
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.86	0.57
1:A:390:LYS:HZ3	1:A:415:GLU:CD	2.11	0.57
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.34	0.57
1:A:173:LYS:O	1:A:176:PRO:HD3	2.04	0.57
2:B:380:ILE:O	2:B:384:GLY:N	2.37	0.57
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.86	0.57
1:A:233:GLU:C	1:A:234:LEU:HD12	2.29	0.57
1:A:92:LEU:HD12	1:A:92:LEU:H	1.69	0.57
1:A:323:LYS:HE3	1:A:344:GLU:HG3	1.87	0.57
1:A:96:HIS:NE2	1:A:350:LYS:HE2	2.19	0.56
2:B:179:VAL:O	2:B:180:ILE:HD12	2.05	0.56
1:A:295:LEU:HD22	1:A:300:GLU:CD	2.30	0.56
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.69	0.56
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.88	0.56
1:A:410:TRP:NE1	2:B:363:ASN:HB2	2.21	0.56
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.88	0.56
2:B:139:THR:HB	2:B:140:PRO:HD2	1.88	0.56
1:A:226:PRO:HA	1:A:234:LEU:O	2.05	0.56
1:A:244:ILE:HG21	1:A:310:LEU:HD13	1.88	0.56
2:B:368:LEU:O	2:B:372:VAL:HG23	2.06	0.56
1:A:500:GLN:OE1	1:A:500:GLN:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LYS:HD2	2:B:424:LYS:O	2.05	0.56
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.88	0.56
1:A:515:SER:CB	1:A:518:VAL:HG23	2.36	0.56
1:A:116:PHE:O	1:A:148:VAL:HG21	2.05	0.55
1:A:27:THR:HG22	1:A:28:GLU:N	2.20	0.55
2:B:101:LYS:NZ	2:B:101:LYS:HB3	2.20	0.55
1:A:95:PRO:HA	2:B:136:ASN:O	2.06	0.55
1:A:6:GLU:CD	1:A:6:GLU:N	2.63	0.55
1:A:441:TYR:HA	1:A:496:VAL:HG13	1.89	0.55
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.36	0.55
2:B:157:PRO:CG	2:B:184:MET:HA	2.33	0.55
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.07	0.55
1:A:92:LEU:HD12	1:A:92:LEU:N	2.22	0.55
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.37	0.55
2:B:254:VAL:HG21	2:B:288:ALA:O	2.07	0.55
1:A:161:GLN:C	1:A:161:GLN:NE2	2.61	0.55
1:A:138:GLU:CG	1:A:139:THR:H	2.07	0.54
2:B:65:LYS:HA	2:B:407:GLN:HG2	1.87	0.54
1:A:25:PRO:O	1:A:26:LEU:HD23	2.06	0.54
1:A:42:GLU:HG3	1:A:144:TYR:HE2	1.72	0.54
1:A:367:GLN:O	1:A:368:LEU:C	2.50	0.54
1:A:402:TRP:HZ3	2:B:364:ASP:OD2	1.90	0.54
2:B:345:PRO:O	2:B:346:PHE:HB2	2.07	0.54
2:B:98:ALA:HB1	2:B:101:LYS:HD3	1.89	0.54
2:B:420:PRO:HB2	2:B:423:VAL:CG1	2.37	0.54
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.88	0.54
2:B:172:ARG:HG3	2:B:172:ARG:HH11	1.72	0.54
1:A:285:GLY:O	1:A:286:THR:C	2.51	0.54
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.07	0.54
1:A:138:GLU:HG3	1:A:139:THR:N	2.14	0.54
1:A:37:ILE:CD1	1:A:72:ARG:HA	2.38	0.54
1:A:125:ARG:CD	1:A:147:ASN:HA	2.29	0.54
1:A:212:TRP:C	1:A:214:LEU:H	2.16	0.54
1:A:344:GLU:O	1:A:345:PRO:C	2.50	0.54
2:B:53:GLU:CD	2:B:53:GLU:H	2.16	0.54
1:A:120:LEU:HD12	1:A:121:ASP:H	1.72	0.54
1:A:248:GLU:HA	1:A:248:GLU:OE2	2.06	0.53
1:A:252:TRP:CD1	1:A:295:LEU:HD12	2.43	0.53
2:B:295:LEU:HD22	2:B:300:GLU:OE2	2.08	0.53
2:B:433:PRO:CG	2:B:436:GLY:HA2	2.38	0.53
1:A:161:GLN:HE21	1:A:162:SER:N	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.23	0.53
1:A:89:GLU:HB2	1:A:92:LEU:HG	1.89	0.53
2:B:291:GLU:HG3	2:B:292:VAL:N	2.22	0.53
2:B:161:GLN:O	2:B:164:MET:HB3	2.08	0.53
2:B:365:VAL:O	2:B:369:THR:HG23	2.09	0.53
2:B:395:LYS:O	2:B:399:GLU:CG	2.52	0.52
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.91	0.52
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.91	0.52
1:A:212:TRP:C	1:A:214:LEU:N	2.65	0.52
2:B:29:GLU:HG2	2:B:30:LYS:N	2.25	0.52
1:A:270:ILE:C	1:A:272:PRO:HD3	2.35	0.52
1:A:283:LEU:O	1:A:286:THR:HG23	2.10	0.52
1:A:206:ARG:NE	1:A:218:ASP:HA	2.24	0.52
1:A:373:GLN:C	1:A:373:GLN:CD	2.78	0.52
1:A:58:THR:HG23	1:A:76:ASP:O	2.09	0.52
1:A:363:ASN:HA	1:A:511:ASP:CG	2.34	0.52
1:A:8:VAL:O	1:A:10:VAL:HG23	2.09	0.52
2:B:205:LEU:C	2:B:205:LEU:HD23	2.35	0.52
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.45	0.52
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.25	0.52
1:A:41:MET:HA	1:A:44:GLU:HB2	1.91	0.52
1:A:109:LEU:HD12	1:A:109:LEU:N	2.25	0.52
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.45	0.52
1:A:505:ILE:O	1:A:509:GLN:N	2.41	0.52
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.91	0.51
1:A:268:SER:HB2	1:A:353:LYS:HD3	1.92	0.51
1:A:333:GLY:HA3	1:A:336:GLN:NE2	2.25	0.51
2:B:63:ILE:HD13	2:B:72:ARG:O	2.10	0.51
2:B:180:ILE:CD1	2:B:189:VAL:HG13	2.39	0.51
2:B:175:ASN:N	2:B:176:PRO:HD3	2.25	0.51
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.39	0.51
2:B:332:GLN:OE1	2:B:424:LYS:HD3	2.10	0.51
1:A:332:GLN:NE2	1:A:332:GLN:HA	2.26	0.51
1:A:516:GLU:O	1:A:520:GLN:HG2	2.11	0.51
1:A:136:ASN:OD1	1:A:138:GLU:CB	2.55	0.51
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.76	0.51
2:B:32:LYS:O	2:B:33:ALA:C	2.52	0.51
2:B:65:LYS:O	2:B:68:SER:HB3	2.11	0.51
2:B:358:ARG:H	2:B:358:ARG:CD	2.24	0.51
1:A:169:GLU:N	1:A:170:PRO:HD2	2.26	0.51
2:B:195:ILE:HG12	2:B:199:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.26	0.51
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.75	0.51
1:A:296:THR:HG23	1:A:299:ALA:CB	2.40	0.50
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.42	0.50
1:A:118:VAL:O	1:A:148:VAL:HG23	2.11	0.50
1:A:2:ILE:HG22	1:A:3:SER:N	2.26	0.50
1:A:136:ASN:O	1:A:137:ASN:C	2.53	0.50
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.94	0.50
1:A:233:GLU:HB3	1:A:240:THR:OG1	2.12	0.50
1:A:250:ASP:OD1	1:A:250:ASP:N	2.44	0.50
1:A:358:ARG:CZ	1:A:358:ARG:CB	2.90	0.50
1:A:216:THR:OG1	1:A:217:PRO:HD2	2.12	0.50
2:B:78:ARG:O	2:B:82:LYS:HG3	2.12	0.50
1:A:136:ASN:O	1:A:138:GLU:N	2.45	0.50
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.46	0.50
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.12	0.50
1:A:448:ARG:HG3	1:A:449:GLU:N	2.27	0.49
2:B:160:PHE:O	2:B:160:PHE:CD1	2.65	0.49
1:A:206:ARG:HG3	1:A:216:THR:HG23	1.93	0.49
1:A:254:VAL:HG21	1:A:288:ALA:O	2.12	0.49
2:B:78:ARG:HD3	2:B:411:ILE:O	2.11	0.49
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.12	0.49
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.94	0.49
2:B:78:ARG:NH1	2:B:412:PRO:O	2.44	0.49
2:B:303:LEU:HD22	2:B:307:ARG:HE	1.77	0.49
1:A:43:LYS:NZ	1:A:44:GLU:HG3	2.27	0.49
1:A:234:LEU:C	1:A:235:HIS:HD2	2.19	0.49
1:A:283:LEU:HA	1:A:286:THR:HG23	1.94	0.49
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.48	0.49
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.47	0.49
1:A:296:THR:O	1:A:299:ALA:HB3	2.12	0.49
1:A:359:GLY:O	1:A:360:ALA:C	2.56	0.49
1:A:151:GLN:HA	1:A:151:GLN:NE2	2.28	0.49
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.94	0.49
2:B:296:THR:HB	2:B:298:GLU:OE2	2.13	0.49
1:A:61:PHE:HB2	1:A:74:LEU:HD23	1.91	0.48
1:A:283:LEU:HA	1:A:286:THR:CG2	2.43	0.48
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.95	0.48
1:A:234:LEU:N	1:A:234:LEU:CD1	2.76	0.48
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.78	0.48
1:A:319:TYR:O	1:A:321:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:413:GLU:C	2.55	0.48
2:B:28:GLU:O	2:B:29:GLU:C	2.56	0.48
1:A:91:GLN:C	1:A:93:GLY:H	2.21	0.48
1:A:106:VAL:HA	1:A:189:VAL:O	2.14	0.48
1:A:168:LEU:O	1:A:172:ARG:HG3	2.13	0.48
1:A:226:PRO:HB2	1:A:233:GLU:HG2	1.95	0.48
1:A:200:THR:O	1:A:203:GLU:HB3	2.14	0.48
2:B:63:ILE:HD13	2:B:63:ILE:N	2.28	0.48
2:B:120:LEU:HD23	2:B:121:ASP:O	2.13	0.48
1:A:249:LYS:HD3	1:A:251:SER:O	2.14	0.48
1:A:418:ASN:O	1:A:420:PRO:HD3	2.14	0.48
1:A:508:ALA:O	1:A:509:GLN:C	2.57	0.48
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.95	0.48
2:B:374:LYS:HA	2:B:374:LYS:HE2	1.95	0.48
1:A:308:GLU:O	1:A:311:LYS:HB2	2.14	0.48
2:B:248:GLU:O	2:B:249:LYS:HD3	2.14	0.48
1:A:92:LEU:H	1:A:92:LEU:CD1	2.26	0.48
1:A:329:ILE:HG22	1:A:330:GLN:N	2.28	0.48
1:A:356:ARG:HH22	1:A:371:ALA:N	2.12	0.48
2:B:350:LYS:HG2	2:B:351:THR:N	2.28	0.48
1:A:465:LYS:HG2	1:A:466:VAL:H	1.79	0.47
1:A:112:GLY:C	1:A:114:ALA:H	2.20	0.47
1:A:168:LEU:O	1:A:172:ARG:CG	2.61	0.47
1:A:209:LEU:O	1:A:214:LEU:HB2	2.14	0.47
1:A:243:PRO:CG	1:A:313:PRO:HB3	2.44	0.47
1:A:515:SER:OG	1:A:518:VAL:HG23	2.14	0.47
2:B:109:LEU:O	2:B:186:ASP:HA	2.14	0.47
2:B:247:PRO:HB2	2:B:249:LYS:HZ1	1.77	0.47
2:B:301:LEU:O	2:B:302:GLU:C	2.57	0.47
1:A:329:ILE:CG2	1:A:330:GLN:N	2.78	0.47
1:A:79:GLU:O	1:A:82:LYS:HB2	2.14	0.47
2:B:366:LYS:HG2	2:B:405:TYR:CD2	2.48	0.47
2:B:75:VAL:HG12	2:B:76:ASP:N	2.30	0.47
2:B:418:ASN:N	2:B:418:ASN:OD1	2.46	0.47
1:A:371:ALA:O	1:A:372:VAL:C	2.57	0.47
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.50	0.47
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.96	0.47
1:A:454:LYS:HA	1:A:467:VAL:O	2.14	0.47
1:A:88:TRP:HD1	2:B:143:ARG:HD3	1.79	0.47
1:A:219:LYS:HA	1:A:222:GLN:CD	2.39	0.47
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLN:HE21	2:B:243:PRO:HD2	1.79	0.47
2:B:126:LYS:HG3	2:B:127:TYR:N	2.30	0.47
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.79	0.47
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.50	0.47
1:A:239:TRP:HZ3	1:A:241:VAL:HG23	1.81	0.46
1:A:438:GLU:HA	1:A:461:ARG:HD2	1.97	0.46
2:B:100:LEU:CD2	2:B:100:LEU:N	2.76	0.46
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.45	0.46
1:A:347:LYS:HA	1:A:347:LYS:HD3	1.66	0.46
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.97	0.46
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.45	0.46
1:A:318:TYR:CE2	3:A:999:NVP:H12	2.51	0.46
1:A:333:GLY:HA3	1:A:336:GLN:HE22	1.78	0.46
1:A:37:ILE:HD11	1:A:72:ARG:HA	1.98	0.46
1:A:136:ASN:C	1:A:138:GLU:N	2.72	0.46
2:B:108:VAL:O	2:B:109:LEU:HD12	2.16	0.46
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.30	0.46
1:A:419:THR:HG23	1:A:419:THR:O	2.16	0.46
1:A:472:THR:OG1	1:A:473:THR:N	2.46	0.46
2:B:280:CYS:C	2:B:284:ARG:HH21	2.23	0.46
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.51	0.46
1:A:484:LEU:O	1:A:487:GLN:HB2	2.16	0.46
2:B:238:LYS:O	2:B:239:TRP:CD1	2.65	0.46
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.46	0.46
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.98	0.46
1:A:235:HIS:CD2	1:A:235:HIS:N	2.84	0.46
1:A:246:LEU:O	1:A:307:ARG:NH1	2.36	0.46
1:A:17:ASP:O	1:A:83:ARG:CD	2.60	0.46
1:A:37:ILE:O	1:A:40:GLU:HB2	2.15	0.46
1:A:253:THR:O	1:A:256:ASP:HB2	2.16	0.46
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.45	0.45
1:A:498:ASP:HA	1:A:536:VAL:O	2.16	0.45
2:B:379:SER:CB	2:B:387:PRO:HD3	2.46	0.45
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.51	0.45
1:A:37:ILE:HG22	1:A:38:CYS:N	2.31	0.45
1:A:142:ILE:N	1:A:142:ILE:CD1	2.80	0.45
1:A:405:TYR:O	2:B:331:LYS:HD3	2.15	0.45
1:A:423:VAL:O	1:A:423:VAL:HG23	2.16	0.45
2:B:303:LEU:HD22	2:B:307:ARG:NE	2.31	0.45
1:A:542:ILE:HD12	1:A:542:ILE:H	1.80	0.45
2:B:201:LYS:O	2:B:204:GLU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:OD1	2:B:363:ASN:C	2.60	0.45
2:B:434:ILE:HG13	2:B:435:VAL:N	2.32	0.45
1:A:252:TRP:CD1	1:A:295:LEU:CD1	2.99	0.45
1:A:416:PHE:HE1	1:A:422:LEU:HD22	1.82	0.45
1:A:541:GLY:HA3	2:B:284:ARG:NH2	2.31	0.45
2:B:383:TRP:O	2:B:384:GLY:C	2.60	0.45
1:A:163:SER:O	1:A:166:LYS:HB2	2.16	0.45
2:B:5:ILE:HG12	2:B:6:GLU:O	2.16	0.45
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.98	0.45
1:A:162:SER:O	1:A:163:SER:C	2.58	0.45
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.81	0.45
1:A:42:GLU:HG3	1:A:144:TYR:CE2	2.50	0.45
1:A:94:ILE:HD11	1:A:183:TYR:CE2	2.51	0.45
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.98	0.45
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.51	0.45
1:A:41:MET:HB2	1:A:46:LYS:HB2	1.98	0.44
1:A:161:GLN:HG2	1:A:182:GLN:OE1	2.17	0.44
1:A:243:PRO:HG3	1:A:313:PRO:CA	2.48	0.44
1:A:292:VAL:C	1:A:293:ILE:HD12	2.42	0.44
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.18	0.44
2:B:162:SER:O	2:B:163:SER:C	2.60	0.44
1:A:3:SER:OG	1:A:5:ILE:HG22	2.17	0.44
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.74	0.44
1:A:249:LYS:CG	1:A:250:ASP:N	2.80	0.44
2:B:52:PRO:O	2:B:53:GLU:C	2.60	0.44
2:B:123:ASP:O	2:B:126:LYS:NZ	2.42	0.44
2:B:185:ASP:HB2	2:B:409:THR:HG21	1.99	0.44
1:A:28:GLU:HG2	1:A:32:LYS:HE3	2.00	0.44
1:A:113:ASP:OD2	1:A:113:ASP:N	2.49	0.44
1:A:262:GLY:O	1:A:263:LYS:C	2.61	0.44
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.46	0.44
2:B:175:ASN:C	2:B:177:ASP:H	2.26	0.44
2:B:195:ILE:CG2	2:B:196:GLY:N	2.80	0.44
1:A:157:PRO:O	1:A:158:ALA:C	2.59	0.44
1:A:457:TYR:CD1	1:A:457:TYR:C	2.95	0.44
2:B:87:PHE:CD1	2:B:87:PHE:N	2.86	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.87	0.44
1:A:376:THR:HG23	1:A:386:THR:HB	1.99	0.44
2:B:31:ILE:O	2:B:35:VAL:HG23	2.18	0.44
1:A:382:ILE:O	2:B:135:ILE:CG2	2.66	0.44
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.81	0.44
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.82	0.44
1:A:357:MET:O	1:A:358:ARG:C	2.60	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
1:A:42:GLU:CG	1:A:144:TYR:CE2	3.00	0.43
1:A:64:LYS:NZ	1:A:69:THR:HG23	2.33	0.43
1:A:161:GLN:O	1:A:164:MET:HB3	2.18	0.43
1:A:340:GLN:CB	1:A:351:THR:HG22	2.48	0.43
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.33	0.43
1:A:475:GLN:O	1:A:479:LEU:HG	2.18	0.43
2:B:104:LYS:CB	2:B:192:ASP:HA	2.48	0.43
1:A:254:VAL:HG13	1:A:286:THR:HG21	2.00	0.43
1:A:357:MET:O	1:A:359:GLY:N	2.51	0.43
1:A:480:GLN:NE2	1:A:484:LEU:HG	2.33	0.43
2:B:52:PRO:C	2:B:54:ASN:N	2.70	0.43
2:B:172:ARG:HH21	2:B:180:ILE:HG22	1.83	0.43
2:B:344:GLU:HB2	2:B:347:LYS:HD2	2.01	0.43
2:B:377:THR:O	2:B:380:ILE:HB	2.19	0.43
1:A:19:PRO:HG3	1:A:80:LEU:HA	2.01	0.43
1:A:94:ILE:HG22	1:A:95:PRO:O	2.18	0.43
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.44	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.27	0.43
2:B:120:LEU:O	2:B:121:ASP:C	2.61	0.43
2:B:237:ASP:C	2:B:239:TRP:N	2.76	0.43
2:B:317:VAL:HG23	2:B:317:VAL:O	2.19	0.43
1:A:69:THR:O	1:A:69:THR:HG22	2.19	0.43
1:A:151:GLN:CA	1:A:151:GLN:HE21	2.31	0.43
1:A:360:ALA:O	1:A:513:SER:HB2	2.18	0.43
1:A:463:ARG:NH1	1:A:488:ASP:O	2.52	0.43
1:A:105:SER:O	1:A:190:GLY:HA2	2.17	0.43
1:A:116:PHE:C	1:A:148:VAL:HG21	2.43	0.43
1:A:340:GLN:HA	1:A:351:THR:HG22	2.00	0.43
1:A:370:GLU:O	1:A:374:LYS:HG3	2.19	0.43
1:A:92:LEU:HD21	2:B:141:GLY:H	1.83	0.43
1:A:219:LYS:HA	1:A:222:GLN:NE2	2.33	0.43
2:B:101:LYS:NZ	2:B:101:LYS:CB	2.82	0.43
2:B:201:LYS:HD2	2:B:201:LYS:HA	1.78	0.43
2:B:245:VAL:CG2	2:B:431:LYS:HB2	2.47	0.43
1:A:150:PRO:HG2	1:A:153:TRP:HB3	2.00	0.43
1:A:293:ILE:HD12	1:A:293:ILE:N	2.34	0.43
1:A:324:ASP:OD2	1:A:324:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ASN:O	2:B:256:ASP:C	2.59	0.43
1:A:5:ILE:HG13	1:A:6:GLU:OE2	2.19	0.43
1:A:219:LYS:HD3	1:A:222:GLN:NE2	2.34	0.43
1:A:474:ASN:O	1:A:475:GLN:C	2.59	0.43
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.19	0.43
2:B:244:ILE:HG23	2:B:429:LEU:HB3	2.01	0.43
1:A:151:GLN:HA	1:A:151:GLN:HE21	1.82	0.43
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.18	0.43
2:B:53:GLU:CD	2:B:53:GLU:N	2.76	0.43
2:B:278:GLN:HB3	2:B:299:ALA:HA	2.01	0.43
2:B:23:GLN:HG3	2:B:24:TRP:O	2.19	0.42
2:B:63:ILE:HD12	2:B:74:LEU:HB2	2.01	0.42
1:A:232:TYR:N	1:A:232:TYR:CD1	2.87	0.42
1:A:249:LYS:HG3	1:A:250:ASP:N	2.34	0.42
2:B:175:ASN:HB3	2:B:178:ILE:HD12	2.00	0.42
1:A:11:LYS:O	1:A:85:GLN:HB3	2.20	0.42
1:A:57:ASN:HA	1:A:129:ALA:O	2.19	0.42
1:A:91:GLN:O	1:A:93:GLY:N	2.49	0.42
1:A:249:LYS:HE3	1:A:249:LYS:HB2	1.67	0.42
2:B:136:ASN:O	2:B:137:ASN:HB2	2.19	0.42
2:B:191:SER:HB2	2:B:193:LEU:HD13	2.00	0.42
2:B:358:ARG:H	2:B:358:ARG:HD2	1.84	0.42
1:A:43:LYS:HZ3	1:A:44:GLU:HG3	1.84	0.42
1:A:194:GLU:HG3	1:A:197:GLN:HG3	2.02	0.42
1:A:240:THR:HG22	1:A:315:HIS:ND1	2.35	0.42
2:B:285:GLY:O	2:B:287:LYS:HG2	2.19	0.42
1:A:478:GLU:O	1:A:481:ALA:HB3	2.19	0.42
2:B:66:LYS:O	2:B:67:ASP:HB2	2.19	0.42
2:B:296:THR:O	2:B:297:GLU:C	2.63	0.42
2:B:435:VAL:HG23	2:B:436:GLY:N	2.35	0.42
1:A:88:TRP:HB3	1:A:89:GLU:OE1	2.20	0.42
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.34	0.42
1:A:110:ASP:O	1:A:217:PRO:HD3	2.19	0.42
1:A:13:LYS:HD2	1:A:82:LYS:O	2.19	0.42
1:A:541:GLY:HA3	2:B:284:ARG:NE	2.34	0.42
2:B:66:LYS:HD2	2:B:66:LYS:HA	1.94	0.42
2:B:78:ARG:NH1	2:B:411:ILE:HG22	2.34	0.42
2:B:101:LYS:HE2	2:B:382:ILE:HG23	2.02	0.42
2:B:242:GLN:HE21	2:B:242:GLN:CA	2.11	0.42
2:B:116:PHE:HA	2:B:148:VAL:HG21	2.02	0.42
1:A:33:ALA:O	1:A:36:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HA	1:A:188:TYR:O	2.20	0.42
1:A:246:LEU:C	1:A:307:ARG:HH12	2.23	0.42
1:A:479:LEU:O	1:A:480:GLN:C	2.62	0.42
1:A:514:GLU:H	1:A:514:GLU:HG3	1.52	0.42
2:B:77:PHE:O	2:B:78:ARG:C	2.62	0.42
2:B:125:ARG:O	2:B:126:LYS:C	2.62	0.42
1:A:205:LEU:O	1:A:206:ARG:C	2.63	0.41
1:A:61:PHE:CB	1:A:74:LEU:HD21	2.38	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.41
2:B:288:ALA:O	2:B:291:GLU:HB3	2.20	0.41
2:B:387:PRO:HG2	2:B:389:PHE:HE1	1.81	0.41
1:A:27:THR:HG22	1:A:29:GLU:H	1.85	0.41
1:A:58:THR:HG23	1:A:59:PRO:HD2	2.02	0.41
1:A:181:TYR:HB3	1:A:188:TYR:HB2	2.02	0.41
1:A:303:LEU:O	1:A:303:LEU:HD23	2.20	0.41
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.20	0.41
1:A:344:GLU:O	1:A:347:LYS:HB2	2.20	0.41
1:A:77:PHE:O	1:A:78:ARG:C	2.61	0.41
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.85	0.41
1:A:27:THR:HG22	1:A:28:GLU:H	1.84	0.41
1:A:111:VAL:HG22	1:A:185:ASP:O	2.20	0.41
1:A:380:ILE:O	1:A:384:GLY:N	2.48	0.41
1:A:408:ALA:O	2:B:393:ILE:HG13	2.21	0.41
1:A:95:PRO:HB3	2:B:136:ASN:O	2.21	0.41
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.41
1:A:154:LYS:O	1:A:157:PRO:HD2	2.21	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.20	0.41
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.94	0.41
2:B:115:TYR:C	2:B:117:SER:H	2.29	0.41
1:A:63:ILE:HG22	1:A:74:LEU:HD22	2.03	0.41
1:A:219:LYS:HD3	1:A:222:GLN:CD	2.46	0.41
1:A:242:GLN:CB	1:A:243:PRO:C	2.94	0.41
1:A:513:SER:OG	1:A:518:VAL:HB	2.21	0.41
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.55	0.41
1:A:205:LEU:O	1:A:208:HIS:N	2.54	0.41
1:A:206:ARG:HH21	1:A:218:ASP:HB3	1.85	0.41
1:A:309:ILE:C	1:A:311:LYS:H	2.28	0.41
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.56	0.41
2:B:35:VAL:O	2:B:36:GLU:C	2.63	0.41
2:B:51:GLY:CA	2:B:53:GLU:OE2	2.68	0.41
2:B:206:ARG:HG2	2:B:210:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HB3	1:A:46:LYS:HE2	2.03	0.41
1:A:101:LYS:O	3:A:999:NVP:H13	2.21	0.41
1:A:480:GLN:HE22	1:A:484:LEU:HG	1.86	0.41
2:B:106:VAL:O	2:B:234:LEU:HB2	2.20	0.41
1:A:134:SER:O	1:A:135:ILE:C	2.64	0.40
1:A:410:TRP:HZ3	2:B:401:TRP:CE2	2.39	0.40
2:B:195:ILE:HG23	2:B:196:GLY:N	2.36	0.40
1:A:99:GLY:HA3	1:A:382:ILE:HG23	2.02	0.40
1:A:356:ARG:HH21	1:A:374:LYS:HZ1	1.69	0.40
2:B:341:ILE:N	2:B:341:ILE:HD12	2.36	0.40
2:B:431:LYS:HG2	2:B:432:GLU:N	2.36	0.40
1:A:2:ILE:HG22	1:A:3:SER:H	1.85	0.40
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.78	0.40
1:A:295:LEU:HD23	1:A:299:ALA:HB3	2.04	0.40
1:A:300:GLU:OE2	1:A:300:GLU:HA	2.20	0.40
1:A:358:ARG:C	1:A:359:GLY:O	2.65	0.40
2:B:180:ILE:HG22	2:B:180:ILE:O	2.21	0.40
1:A:118:VAL:O	1:A:148:VAL:CG2	2.69	0.40
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.50	0.40
1:A:356:ARG:NH1	1:A:367:GLN:HB3	2.36	0.40
1:A:418:ASN:O	1:A:418:ASN:CG	2.62	0.40
2:B:345:PRO:O	2:B:346:PHE:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/543 (99%)	470 (87%)	49 (9%)	20 (4%)	2	11
2	B	402/440 (91%)	349 (87%)	47 (12%)	6 (2%)	8	28
All	All	941/983 (96%)	819 (87%)	96 (10%)	26 (3%)	4	15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
1	A	242	GLN
2	B	162	SER
1	A	88	TRP
1	A	91	GLN
1	A	92	LEU
1	A	137	ASN
1	A	230	MET
1	A	358	ARG
2	B	361	HIS
1	A	18	GLY
1	A	68	SER
1	A	250	ASP
1	A	360	ALA
2	B	267	ALA
2	B	238	LYS
1	A	4	PRO
1	A	69	THR
1	A	85	GLN
1	A	286	THR
1	A	310	LEU
1	A	345	PRO
1	A	236	PRO
1	A	195	ILE
2	B	167	ILE
2	B	236	PRO

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	485/485 (100%)	429 (88%)	56 (12%)	5	18
2	B	370/400 (92%)	333 (90%)	37 (10%)	7	24
All	All	855/885 (97%)	762 (89%)	93 (11%)	6	20

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	6	GLU
1	A	11	LYS
1	A	21	VAL
1	A	22	LYS
1	A	37	ILE
1	A	40	GLU
1	A	42	GLU
1	A	88	TRP
1	A	89	GLU
1	A	92	LEU
1	A	105	SER
1	A	122	GLU
1	A	161	GLN
1	A	168	LEU
1	A	182	GLN
1	A	184	MET
1	A	189	VAL
1	A	194	GLU
1	A	205	LEU
1	A	211	ARG
1	A	215	THR
1	A	216	THR
1	A	219	LYS
1	A	228	LEU
1	A	230	MET
1	A	238	LYS
1	A	250	ASP
1	A	253	THR
1	A	264	LEU
1	A	279	LEU
1	A	295	LEU
1	A	296	THR
1	A	303	LEU
1	A	312	GLU
1	A	336	GLN
1	A	340	GLN
1	A	349	LEU
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	369	THR

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Mol	Chain	Res	Type
1	A	374	LYS
1	A	386	THR
1	A	388	LYS
1	A	424	LYS
1	A	449	GLU
1	A	475	GLN
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	514	GLU
1	A	517	LEU
1	A	527	LYS
1	A	540	LYS
2	B	6	GLU
2	B	8	VAL
2	B	24	TRP
2	B	29	GLU
2	B	55	PRO
2	B	63	ILE
2	B	65	LYS
2	B	69	THR
2	B	87	PHE
2	B	100	LEU
2	B	103	ASN
2	B	123	ASP
2	B	134	SER
2	B	161	GLN
2	B	162	SER
2	B	163	SER
2	B	179	VAL
2	B	180	ILE
2	B	186	ASP
2	B	194	GLU
2	B	236	PRO
2	B	237	ASP
2	B	242	GLN
2	B	281	LYS
2	B	283	LEU
2	B	284	ARG
2	B	287	LYS
2	B	289	LEU

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Mol	Chain	Res	Type
2	B	291	GLU
2	B	358	ARG
2	B	362	THR
2	B	363	ASN
2	B	366	LYS
2	B	368	LEU
2	B	381	VAL
2	B	418	ASN
2	B	423	VAL

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	23	GLN
1	A	103	ASN
1	A	137	ASN
1	A	151	GLN
1	A	161	GLN
1	A	197	GLN
1	A	207	GLN
1	A	278	GLN
1	A	332	GLN
1	A	336	GLN
1	A	367	GLN
1	A	475	GLN
1	A	480	GLN
1	A	512	GLN
2	B	57	ASN
2	B	85	GLN
2	B	147	ASN
2	B	151	GLN
2	B	242	GLN
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.81	1 (25%)	1,8,10	2.22	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	3.32	1.50	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	2.22	109.69	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	NVP	A	999	-	23,23,23	1.49	4 (17%)	34,34,34	2.15	6 (17%)

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	NVP	A	999	-	-	0/4/6/6	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C10-C9	4.30	1.54	1.49
3	A	999	NVP	C15-N1	2.45	1.44	1.42
3	A	999	NVP	C10-C15	2.33	1.43	1.40
3	A	999	NVP	C7-N8	2.15	1.44	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	C7-C2-N1	-6.86	117.51	120.14
3	A	999	NVP	C7-N8-C9	6.79	133.89	128.29
3	A	999	NVP	N3-C2-N1	4.47	120.04	116.67
3	A	999	NVP	N14-C15-N1	3.35	119.20	116.67
3	A	999	NVP	C15-C10-C9	-2.25	121.81	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	C10-C15-N1	-2.20	118.21	120.95

There are no chirality outliers.

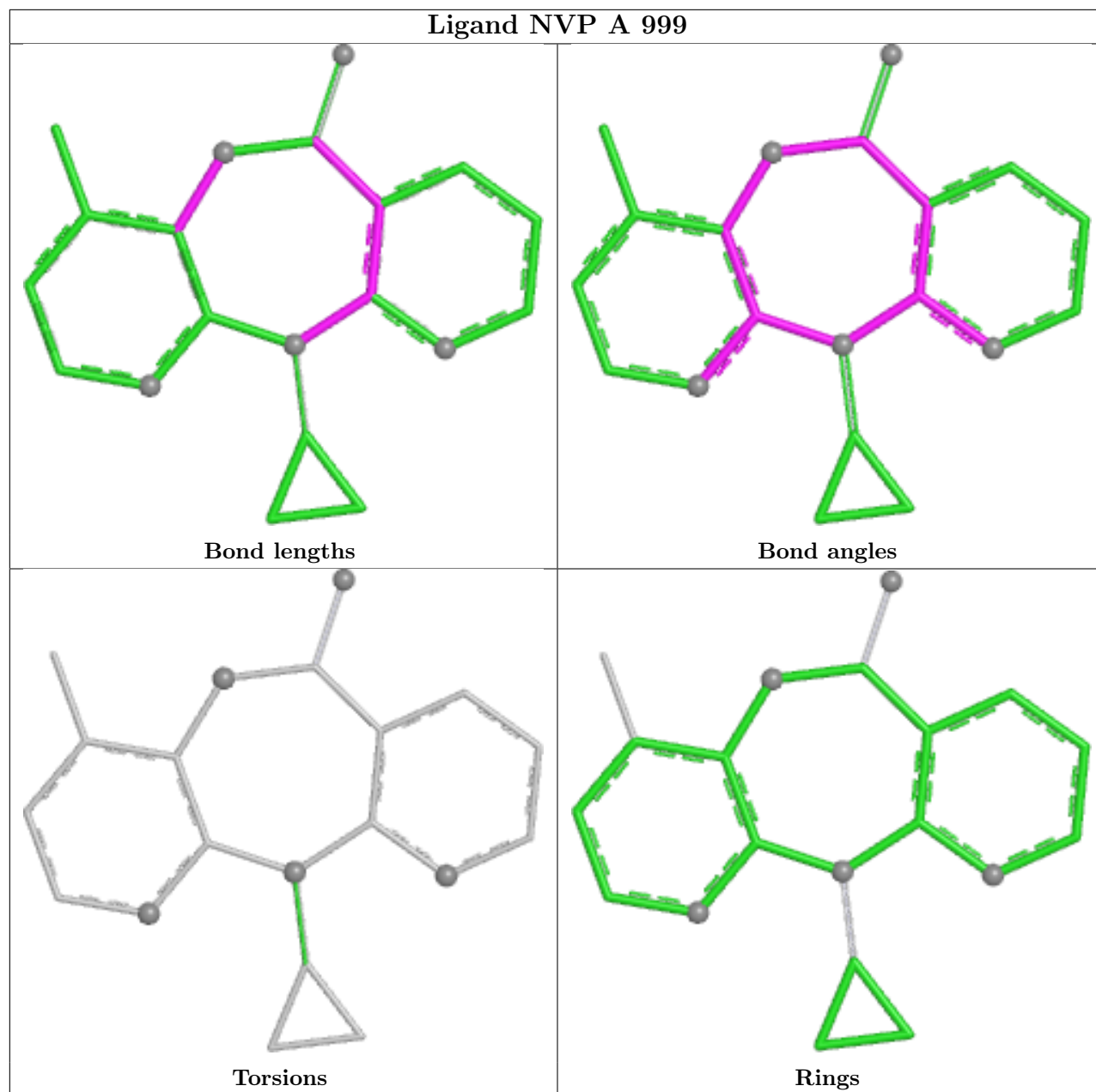
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	NVP	2	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	541/543 (99%)	-0.11	5 (0%) 81 75	20, 63, 127, 150	0
2	B	408/440 (92%)	-0.22	2 (0%) 87 83	23, 62, 114, 149	0
All	All	949/983 (96%)	-0.16	7 (0%) 84 79	20, 63, 122, 150	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	435	VAL	3.7
2	B	87	PHE	2.9
1	A	219	LYS	2.8
1	A	90	VAL	2.7
1	A	1	PRO	2.3
1	A	24	TRP	2.3
1	A	133	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.96	0.07	36,64,80,84	0

6.3 Carbohydrates [i](#)

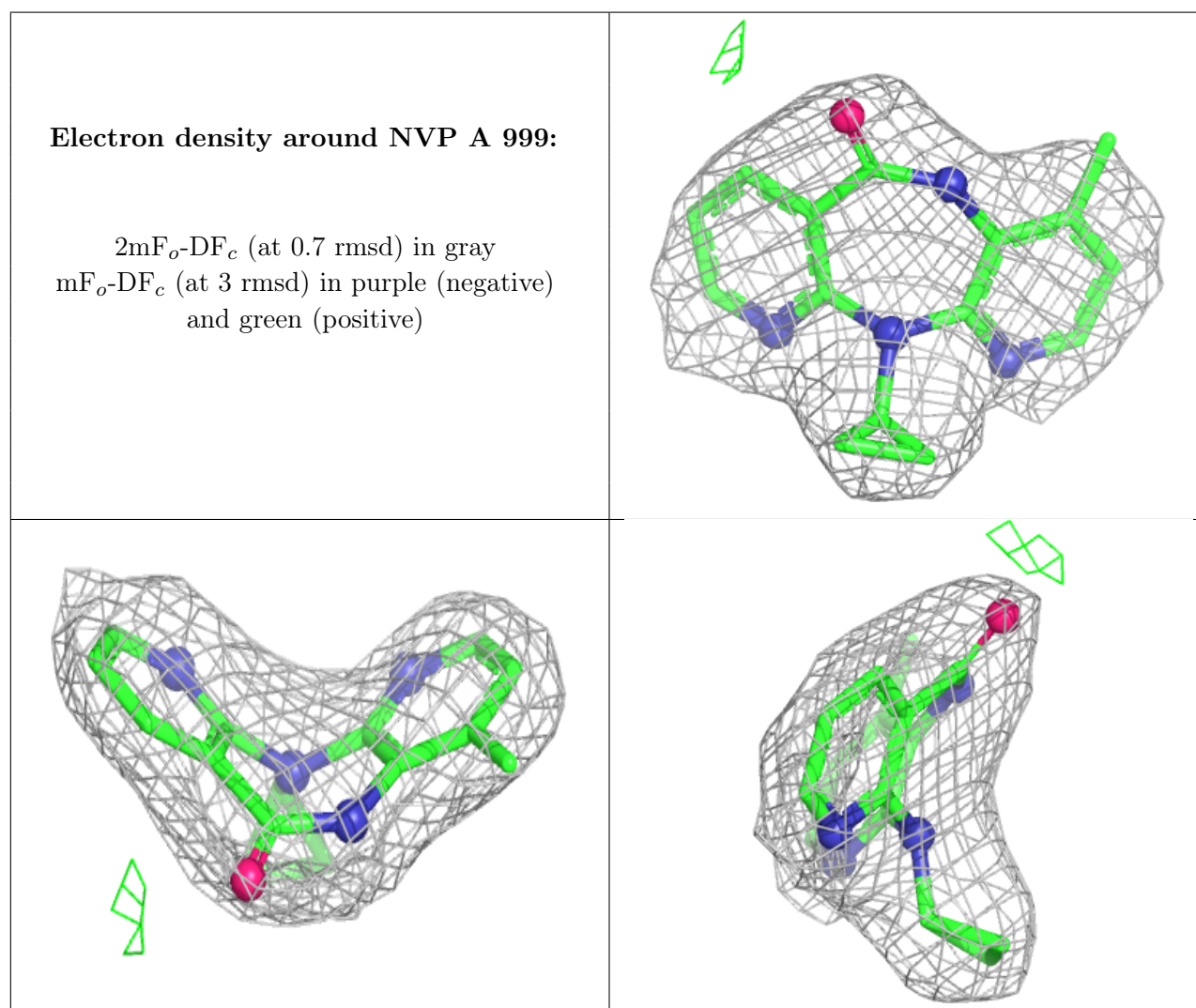
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NVP	A	999	20/20	0.93	0.09	34,54,73,76	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.