



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:19 AM UTC

PDB ID : 2OPR / pdb_00002opr
Title : Crystal Structure of K101E Mutant HIV-1 Reverse Transcriptase in Complex with GW420867X.
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Weaver, K.L.; Short, S.A.; Chan, J.H.; Kleim, J.; Stammers, D.K.
Deposited on : 2007-01-30
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

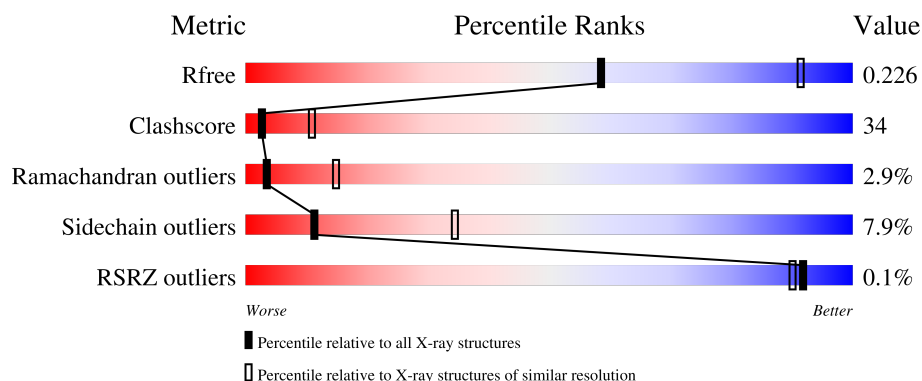
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

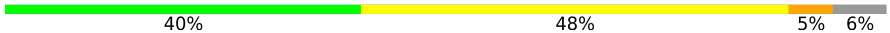
The reported resolution of this entry is 2.90 Å.

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))
R_{free}	180053	2481 (2.90-2.90)
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	547	 37% 50% 10% ..
2	B	426	 40% 48% 5% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7734 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4401	2845	733	815	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLU	LYS	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

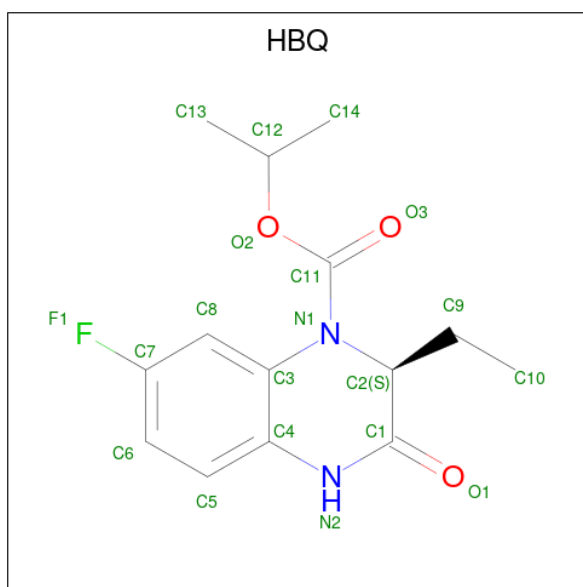
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3313	2151	551	604	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	101	GLU	LYS	engineered mutation	UNP P04585

- Molecule 3 is ISOPROPYL (2S)-2-ETHYL-7-FLUORO-3-OXO-3,4-DIHYDROQUINOXALINE-1(2H)-CARBOXYLATE (CCD ID: HBQ) (formula: C₁₄H₁₇FN₂O₃).

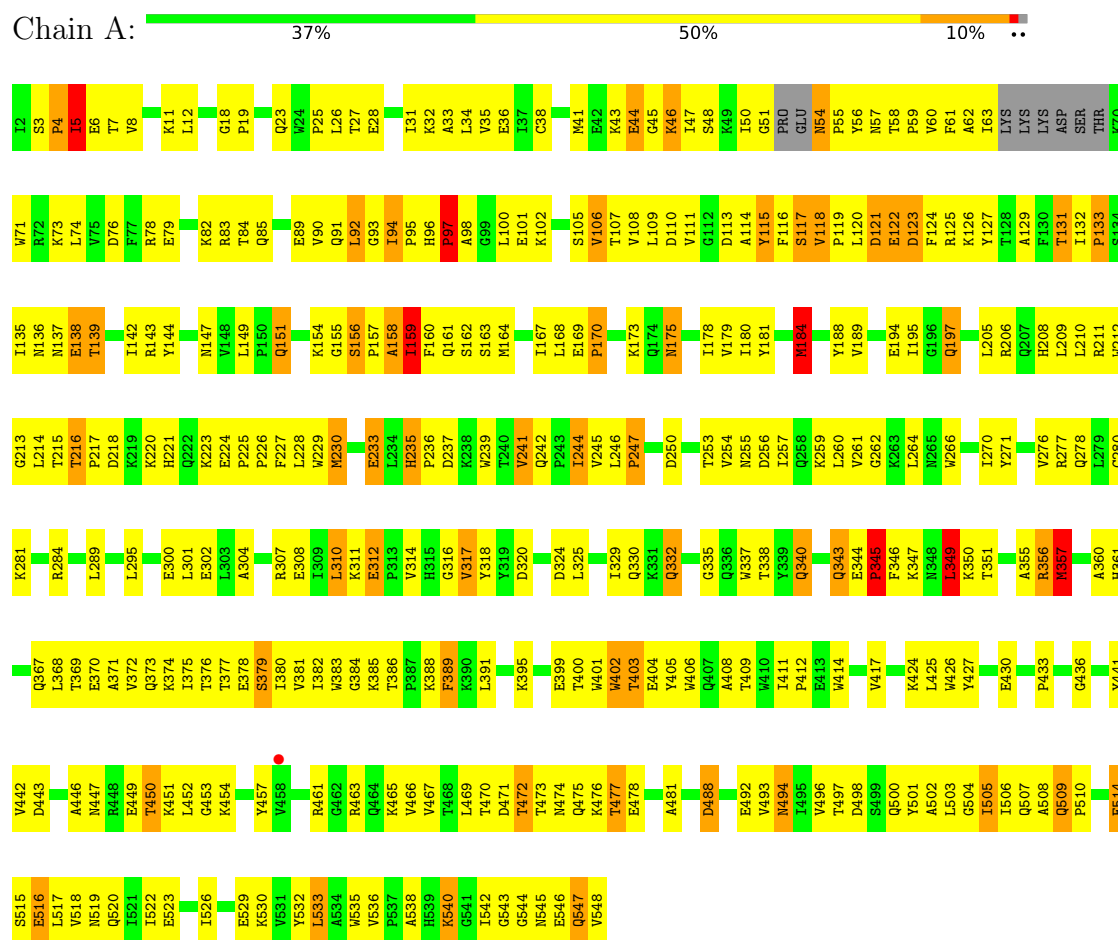


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	20	14	1	2	3	0	0

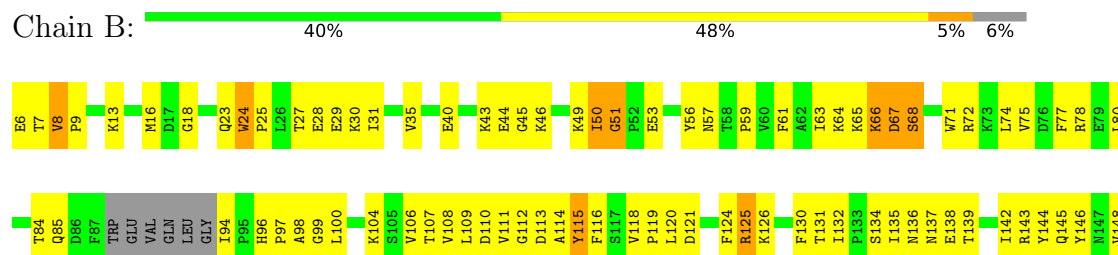
3 Residue-property plots

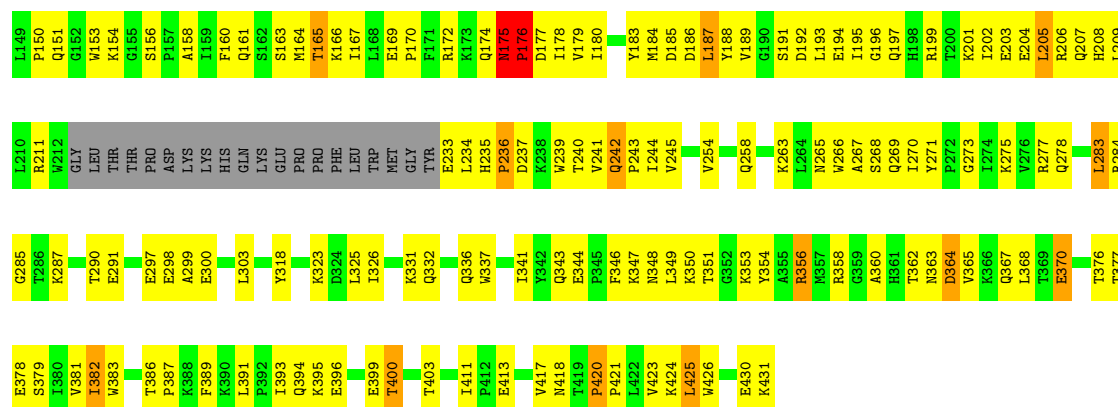
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.00Å 109.30Å 72.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.90 29.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.48-2.90) 96.2 (29.48-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.303 0.215 , 0.226	Depositor DCC
R_{free} test set	1160 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 103.4	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	0.95	EDS
Total number of atoms	7734	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: HBQ, CSD

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	0.66	0/4506	1.16	38/6123 (0.6%)
2	B	0.66	0/3404	1.17	32/4620 (0.7%)
All	All	0.66	0/7910	1.17	70/10743 (0.7%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ILE	N-CA-C	10.12	123.04	109.37
2	B	67	ASP	N-CA-C	9.91	124.67	112.58
1	A	135	ILE	N-CA-C	-9.35	101.28	110.72
2	B	175	ASN	CA-C-N	9.03	131.12	119.84
2	B	175	ASN	C-N-CA	9.03	131.12	119.84
1	A	349	LEU	N-CA-C	-8.94	102.14	113.23
2	B	68	SER	N-CA-C	8.92	124.00	109.72
2	B	241	VAL	N-CA-C	-8.25	96.33	108.87
1	A	547	GLN	N-CA-C	-8.24	101.56	111.69
1	A	235	HIS	N-CA-C	-8.07	99.82	110.40
2	B	382	ILE	N-CA-C	7.55	118.47	111.45
1	A	224	GLU	CA-C-N	7.40	128.00	120.38
1	A	224	GLU	C-N-CA	7.40	128.00	120.38
1	A	509	GLN	CA-C-N	7.20	127.77	119.99
1	A	509	GLN	C-N-CA	7.20	127.77	119.99
1	A	89	GLU	N-CA-C	7.07	120.21	110.24
2	B	51	GLY	CA-C-N	6.86	126.49	119.56
2	B	51	GLY	C-N-CA	6.86	126.49	119.56
2	B	186	ASP	N-CA-C	6.83	120.62	110.52
2	B	343	GLN	N-CA-C	-6.72	105.71	114.04
1	A	54	ASN	CA-C-N	6.62	126.07	118.85
1	A	54	ASN	C-N-CA	6.62	126.07	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLU	N-CA-C	-6.47	98.69	109.24
1	A	343	GLN	N-CA-C	-6.41	106.09	114.04
1	A	350	LYS	N-CA-C	6.40	118.87	108.76
2	B	242	GLN	N-CA-C	6.38	118.75	110.40
2	B	348	ASN	N-CA-C	6.36	118.98	109.25
2	B	115	TYR	N-CA-C	6.22	118.86	111.33
2	B	360	ALA	N-CA-C	-6.14	104.19	113.89
1	A	25	PRO	N-CA-C	-6.03	100.91	112.01
2	B	285	GLY	N-CA-C	-6.03	103.11	112.45
1	A	131	THR	N-CA-C	6.01	119.30	108.48
2	B	175	ASN	N-CA-C	6.01	123.09	109.81
2	B	417	VAL	N-CA-C	5.99	117.33	108.65
2	B	420	PRO	N-CA-C	-5.91	103.50	110.70
2	B	235	HIS	CA-C-N	5.89	127.21	119.84
2	B	235	HIS	C-N-CA	5.89	127.21	119.84
1	A	118	VAL	N-CA-C	5.85	114.57	107.61
1	A	508	ALA	N-CA-C	-5.85	106.05	112.72
1	A	449	GLU	N-CA-C	5.82	118.85	111.69
1	A	175	ASN	CA-C-N	5.80	125.48	119.56
1	A	175	ASN	C-N-CA	5.80	125.48	119.56
1	A	357	MET	N-CA-C	-5.77	101.50	110.10
1	A	184	MET	CB-CA-C	-5.77	109.94	116.63
2	B	8	VAL	CA-C-N	5.73	127.00	119.84
2	B	8	VAL	C-N-CA	5.73	127.00	119.84
1	A	391	LEU	N-CA-C	5.71	118.75	110.14
2	B	391	LEU	N-CA-C	5.67	117.85	109.62
1	A	494	ASN	N-CA-C	-5.64	99.83	109.24
2	B	269	GLN	N-CA-C	-5.58	106.42	113.18
1	A	514	GLU	N-CA-C	-5.57	104.60	111.40
2	B	50	ILE	N-CA-C	5.53	118.07	108.95
1	A	509	GLN	N-CA-C	5.33	121.60	109.81
1	A	250	ASP	N-CA-C	-5.32	106.96	113.50
1	A	215	THR	N-CA-C	5.29	117.59	109.07
1	A	360	ALA	N-CA-C	-5.28	106.97	113.41
2	B	125	ARG	N-CA-C	5.27	117.44	111.11
2	B	175	ASN	C-N-CD	-5.27	103.40	125.00
2	B	176	PRO	CA-N-CD	-5.26	104.64	112.00
1	A	388	LYS	N-CA-C	-5.23	100.77	109.46
1	A	389	PHE	N-CA-C	5.21	118.11	109.46
2	B	237	ASP	N-CA-C	5.21	120.29	113.20
1	A	197	GLN	N-CA-C	-5.15	104.93	111.11
1	A	92	LEU	N-CA-C	-5.12	107.03	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	THR	N-CA-C	5.08	117.71	111.82
1	A	225	PRO	N-CA-C	-5.08	104.51	110.70
1	A	245	VAL	N-CA-C	5.06	115.97	108.23
2	B	365	VAL	N-CA-C	5.06	115.78	110.62
2	B	363	ASN	N-CA-C	5.03	118.35	107.49
2	B	349	LEU	N-CA-C	-5.01	105.92	112.23

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	4401	0	4429	340	1
2	B	3313	0	3342	197	1
3	A	20	0	17	5	0
All	All	7734	0	7788	522	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 34.

All (522) 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:175:ASN:HB3	1:A:178:ILE:HD12	1.32	1.09
1:A:5:ILE:HD13	1:A:5:ILE:H	1.24	1.02
2:B:197:GLN:HB3	2:B:201:LYS:HE2	1.48	0.94
2:B:350:LYS:HE3	2:B:378:GLU:OE1	1.68	0.93
1:A:57:ASN:HD22	1:A:143:ARG:NH2	1.68	0.89
1:A:57:ASN:HD21	1:A:131:THR:HG22	1.36	0.89
1:A:277:ARG:NH1	1:A:277:ARG:HB2	1.90	0.87
2:B:163:SER:O	2:B:167:ILE:HG23	1.75	0.86
2:B:195:ILE:HD11	2:B:199:ARG:NH2	1.91	0.85
1:A:451:LYS:O	1:A:471:ASP:N	2.11	0.84
2:B:239:TRP:HB3	2:B:350:LYS:HE2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD13	1:A:94:ILE:H	1.44	0.81
1:A:501:TYR:CE2	1:A:505:ILE:HD12	2.17	0.80
1:A:277:ARG:HB2	1:A:277:ARG:HH11	1.46	0.79
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.29	0.79
1:A:277:ARG:HH11	1:A:277:ARG:CB	1.96	0.79
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.63	0.78
1:A:181:TYR:HD1	3:A:999:HBQ:H12	1.47	0.78
1:A:123:ASP:O	1:A:126:LYS:HE2	1.84	0.78
2:B:108:VAL:HG22	2:B:188:TYR:CE1	2.19	0.77
1:A:543:GLY:HA3	2:B:283:LEU:O	1.83	0.77
2:B:240:THR:O	2:B:350:LYS:HG3	1.83	0.77
1:A:5:ILE:H	1:A:5:ILE:CD1	1.93	0.77
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.49	0.77
1:A:451:LYS:HE3	1:A:471:ASP:OD2	1.85	0.77
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.49	0.76
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.64	0.76
2:B:194:GLU:OE1	2:B:197:GLN:HG3	1.86	0.75
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.21	0.74
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.21	0.74
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.22	0.73
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.70	0.73
1:A:149:LEU:HD21	1:A:159:ILE:CG2	2.18	0.73
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.71	0.72
1:A:23:GLN:HG3	1:A:133:PRO:HG3	1.69	0.72
1:A:501:TYR:CD2	1:A:505:ILE:HD12	2.24	0.72
1:A:443:ASP:OD2	1:A:548:VAL:HB	1.89	0.72
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.86	0.72
1:A:436:GLY:O	1:A:461:ARG:NH2	2.23	0.72
1:A:206:ARG:NH1	1:A:216:THR:HB	2.04	0.71
1:A:106:VAL:HG23	1:A:236:PRO:HB3	1.72	0.71
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.72	0.70
2:B:197:GLN:HB3	2:B:201:LYS:CE	2.21	0.70
1:A:454:LYS:HA	1:A:467:VAL:O	1.91	0.70
2:B:239:TRP:CE3	2:B:378:GLU:HG3	2.26	0.70
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.91	0.70
1:A:380:ILE:HG22	2:B:25:PRO:HB2	1.72	0.69
1:A:58:THR:HG23	1:A:76:ASP:O	1.93	0.69
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.75	0.69
1:A:409:THR:O	2:B:364:ASP:HB2	1.92	0.69
2:B:31:ILE:O	2:B:35:VAL:HG23	1.93	0.68
2:B:424:LYS:HD2	2:B:425:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.28	0.68
2:B:108:VAL:HG22	2:B:188:TYR:CD1	2.28	0.68
1:A:301:LEU:C	1:A:301:LEU:HD23	2.18	0.68
1:A:50:ILE:O	1:A:143:ARG:HB2	1.93	0.68
1:A:270:ILE:CG2	1:A:314:VAL:HG11	2.23	0.68
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.77	0.67
1:A:443:ASP:CB	1:A:548:VAL:HG11	2.23	0.67
2:B:172:ARG:O	2:B:176:PRO:HD3	1.94	0.67
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.30	0.67
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.76	0.67
2:B:239:TRP:O	2:B:240:THR:HG23	1.95	0.67
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.75	0.67
1:A:57:ASN:HD21	1:A:131:THR:CG2	2.08	0.67
1:A:57:ASN:ND2	1:A:131:THR:HG22	2.09	0.67
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.76	0.67
1:A:57:ASN:ND2	1:A:143:ARG:HH21	1.94	0.66
2:B:29:GLU:OE1	2:B:71:TRP:CZ2	2.48	0.66
1:A:184:MET:HE3	1:A:184:MET:HA	1.76	0.66
1:A:244:ILE:HB	1:A:310:LEU:CD1	2.26	0.66
2:B:84:THR:HB	2:B:154:LYS:HE2	1.77	0.66
1:A:5:ILE:HD13	1:A:5:ILE:N	2.07	0.65
2:B:179:VAL:O	2:B:189:VAL:HA	1.97	0.65
1:A:451:LYS:HA	1:A:472:THR:O	1.96	0.65
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.31	0.65
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.31	0.65
1:A:340:GLN:CB	1:A:351:THR:HG22	2.27	0.65
1:A:493:VAL:HG22	1:A:494:ASN:N	2.12	0.65
2:B:29:GLU:OE1	2:B:71:TRP:HZ2	1.79	0.65
2:B:287:LYS:HD3	2:B:291:GLU:OE1	1.96	0.65
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.32	0.65
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.25	0.65
1:A:100:LEU:HD23	2:B:138:GLU:OE1	1.97	0.65
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.32	0.64
1:A:4:PRO:HB2	1:A:5:ILE:HD13	1.78	0.64
1:A:79:GLU:O	1:A:83:ARG:HD2	1.97	0.64
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.78	0.64
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.20	0.64
1:A:91:GLN:HG3	1:A:93:GLY:O	1.98	0.64
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.33	0.64
1:A:181:TYR:CD1	3:A:999:HBQ:H12	2.31	0.63
1:A:349:LEU:HD12	1:A:383:TRP:CZ2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:O	1:A:522:ILE:HG13	1.98	0.63
1:A:540:LYS:HB3	1:A:542:ILE:HG13	1.80	0.63
2:B:244:ILE:HD12	2:B:430:GLU:HG2	1.81	0.63
2:B:421:PRO:O	2:B:425:LEU:HD13	1.99	0.63
1:A:107:THR:HG22	1:A:108:VAL:H	1.63	0.63
1:A:116:PHE:CZ	1:A:151:GLN:HB2	2.34	0.63
1:A:443:ASP:HB2	1:A:548:VAL:HG11	1.80	0.63
1:A:505:ILE:O	1:A:510:PRO:CD	2.47	0.63
2:B:239:TRP:HE3	2:B:382:ILE:HD11	1.64	0.62
1:A:370:GLU:O	1:A:373:GLN:HG3	1.99	0.62
1:A:478:GLU:O	1:A:481:ALA:HB3	1.98	0.62
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.15	0.62
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.34	0.62
1:A:136:ASN:O	1:A:138:GLU:N	2.33	0.62
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.35	0.62
1:A:346:PHE:N	1:A:346:PHE:CD2	2.67	0.62
2:B:254:VAL:O	2:B:258:GLN:HG3	2.00	0.61
1:A:247:PRO:O	1:A:307:ARG:NH2	2.29	0.61
1:A:379:SER:HB3	1:A:383:TRP:CE3	2.35	0.61
2:B:174:GLN:O	2:B:174:GLN:HG2	2.00	0.61
1:A:206:ARG:HH11	1:A:216:THR:HB	1.65	0.61
1:A:107:THR:HG22	1:A:108:VAL:N	2.15	0.61
1:A:380:ILE:O	1:A:384:GLY:HA2	2.01	0.61
1:A:5:ILE:O	1:A:119:PRO:HG3	2.01	0.61
1:A:122:GLU:H	1:A:122:GLU:CD	2.09	0.60
1:A:132:ILE:HB	1:A:142:ILE:HB	1.83	0.60
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.83	0.60
2:B:396:GLU:O	2:B:400:THR:HG23	2.02	0.60
1:A:514:GLU:HG3	1:A:515:SER:N	2.17	0.60
1:A:3:SER:OG	1:A:4:PRO:HD2	2.02	0.60
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.16	0.60
2:B:233:GLU:HA	2:B:233:GLU:OE2	2.01	0.60
1:A:110:ASP:O	1:A:217:PRO:HD3	2.02	0.60
1:A:451:LYS:HB3	1:A:472:THR:N	2.16	0.59
1:A:402:TRP:CH2	2:B:362:THR:HA	2.37	0.59
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.85	0.59
1:A:94:ILE:H	1:A:94:ILE:CD1	2.16	0.59
1:A:159:ILE:HG22	1:A:160:PHE:N	2.16	0.59
2:B:191:SER:HB2	2:B:193:LEU:HD12	1.85	0.59
2:B:195:ILE:HG23	2:B:196:GLY:N	2.18	0.59
1:A:377:THR:O	1:A:381:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG23	2:B:196:GLY:H	1.66	0.59
1:A:23:GLN:CG	1:A:133:PRO:HG3	2.33	0.59
1:A:218:ASP:N	1:A:221:HIS:HD2	2.00	0.59
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.03	0.58
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.85	0.58
1:A:335:GLY:O	1:A:356:ARG:HA	2.04	0.58
2:B:344:GLU:CB	2:B:347:LYS:HD2	2.34	0.58
1:A:503:LEU:O	1:A:507:GLN:HB3	2.04	0.57
2:B:267:ALA:CB	2:B:426:TRP:CH2	2.87	0.57
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.49	0.57
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.04	0.57
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.85	0.57
1:A:218:ASP:H	1:A:221:HIS:HD2	1.52	0.57
2:B:74:LEU:HD12	2:B:75:VAL:N	2.18	0.57
1:A:51:GLY:HA2	1:A:143:ARG:HD3	1.87	0.57
1:A:475:GLN:OE1	1:A:501:TYR:CZ	2.58	0.57
1:A:505:ILE:O	1:A:510:PRO:HG2	2.04	0.57
2:B:6:GLU:HG2	2:B:6:GLU:O	2.04	0.57
1:A:324:ASP:O	1:A:343:GLN:HG2	2.03	0.57
1:A:357:MET:HE1	1:A:374:LYS:HE3	1.86	0.57
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.40	0.57
2:B:94:ILE:HG13	2:B:94:ILE:O	2.05	0.57
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.85	0.57
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.40	0.57
1:A:443:ASP:HB3	1:A:548:VAL:CG1	2.35	0.57
1:A:443:ASP:HB3	1:A:548:VAL:HG11	1.87	0.57
1:A:500:GLN:NE2	1:A:535:TRP:CZ2	2.73	0.57
1:A:229:TRP:O	1:A:230:MET:C	2.47	0.56
1:A:501:TYR:CE2	1:A:505:ILE:CD1	2.86	0.56
2:B:197:GLN:O	2:B:201:LYS:HG3	2.05	0.56
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.87	0.56
1:A:516:GLU:O	1:A:519:ASN:HB2	2.05	0.56
2:B:74:LEU:HD12	2:B:75:VAL:H	1.70	0.56
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.24	0.56
1:A:379:SER:HB3	1:A:383:TRP:HE3	1.71	0.56
2:B:376:THR:CG2	2:B:386:THR:HG22	2.35	0.56
1:A:246:LEU:O	1:A:307:ARG:NH1	2.38	0.56
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.41	0.56
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.87	0.56
1:A:184:MET:HA	1:A:184:MET:CE	2.36	0.56
1:A:255:ASN:O	1:A:259:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD21	1:A:159:ILE:HG22	1.89	0.55
1:A:452:LEU:HD21	1:A:470:THR:HG22	1.87	0.55
1:A:295:LEU:HB2	1:A:300:GLU:OE1	2.06	0.55
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.88	0.55
2:B:263:LYS:HE3	2:B:425:LEU:HB3	1.88	0.55
2:B:268:SER:HA	2:B:271:TYR:O	2.06	0.55
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.87	0.55
1:A:136:ASN:C	1:A:138:GLU:N	2.62	0.55
1:A:228:LEU:HD22	1:A:242:GLN:OE1	2.07	0.55
1:A:19:PRO:O	1:A:56:TYR:HA	2.07	0.54
1:A:208:HIS:O	1:A:212:TRP:HD1	1.90	0.54
1:A:301:LEU:HD23	1:A:302:GLU:N	2.22	0.54
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.87	0.54
1:A:168:LEU:O	1:A:169:GLU:C	2.51	0.54
1:A:241:VAL:HG23	1:A:314:VAL:O	2.07	0.54
1:A:78:ARG:O	1:A:82:LYS:HG3	2.07	0.54
1:A:96:HIS:O	1:A:97:PRO:C	2.51	0.54
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.08	0.54
1:A:519:ASN:O	1:A:523:GLU:HG2	2.07	0.54
1:A:257:ILE:O	1:A:261:VAL:HG23	2.08	0.54
1:A:136:ASN:C	1:A:138:GLU:H	2.16	0.54
1:A:540:LYS:H	1:A:545:ASN:ND2	2.05	0.54
1:A:169:GLU:O	1:A:173:LYS:HG3	2.09	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.96	0.53
1:A:371:ALA:O	1:A:375:ILE:HG13	2.09	0.53
2:B:64:LYS:HG3	2:B:71:TRP:CE3	2.44	0.53
1:A:62:ALA:C	1:A:63:ILE:HD12	2.34	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.96	0.53
1:A:516:GLU:O	1:A:520:GLN:HG3	2.08	0.53
2:B:158:ALA:C	2:B:160:PHE:N	2.66	0.53
1:A:357:MET:HE1	1:A:374:LYS:CE	2.39	0.53
1:A:97:PRO:HD3	1:A:229:TRP:HD1	1.74	0.53
1:A:427:TYR:C	1:A:427:TYR:CD2	2.87	0.53
2:B:65:LYS:NZ	2:B:110:ASP:OD1	2.42	0.53
2:B:234:LEU:HD13	2:B:381:VAL:HG21	1.91	0.53
1:A:465:LYS:HG2	1:A:466:VAL:N	2.24	0.52
1:A:540:LYS:C	1:A:542:ILE:H	2.15	0.52
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.44	0.52
1:A:23:GLN:CD	1:A:60:VAL:HG12	2.34	0.52
1:A:161:GLN:O	1:A:164:MET:HB3	2.09	0.52
1:A:277:ARG:NH1	1:A:277:ARG:CB	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.56	0.52
2:B:379:SER:CB	2:B:387:PRO:HD3	2.38	0.52
1:A:27:THR:O	1:A:31:ILE:HG13	2.09	0.52
1:A:451:LYS:CE	1:A:471:ASP:OD2	2.55	0.52
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.24	0.52
2:B:326:ILE:O	2:B:341:ILE:HA	2.09	0.52
1:A:26:LEU:HD12	1:A:133:PRO:HG2	1.91	0.52
1:A:493:VAL:CG2	1:A:494:ASN:N	2.73	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.10	0.52
1:A:114:ALA:HA	1:A:117:SER:HB2	1.92	0.52
1:A:244:ILE:HD12	1:A:310:LEU:HD13	1.91	0.52
1:A:357:MET:CE	1:A:374:LYS:HE3	2.40	0.52
2:B:277:ARG:NH2	2:B:278:GLN:OE1	2.43	0.51
1:A:522:ILE:O	1:A:526:ILE:HG13	2.10	0.51
1:A:254:VAL:HB	1:A:289:LEU:O	2.10	0.51
2:B:120:LEU:O	2:B:121:ASP:C	2.53	0.51
1:A:329:ILE:HG22	1:A:330:GLN:N	2.25	0.51
1:A:44:GLU:OE1	1:A:46:LYS:HE2	2.10	0.51
1:A:505:ILE:O	1:A:510:PRO:CG	2.58	0.51
2:B:97:PRO:O	2:B:99:GLY:N	2.44	0.51
1:A:497:THR:O	1:A:535:TRP:HA	2.10	0.51
1:A:344:GLU:O	1:A:345:PRO:C	2.54	0.51
1:A:545:ASN:HA	1:A:548:VAL:HG22	1.93	0.51
2:B:161:GLN:O	2:B:165:THR:HG22	2.11	0.51
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.92	0.51
1:A:408:ALA:O	2:B:393:ILE:HG13	2.11	0.51
1:A:417:VAL:O	1:A:417:VAL:HG13	2.11	0.50
1:A:452:LEU:HA	1:A:469:LEU:O	2.11	0.50
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.21	0.50
1:A:503:LEU:O	1:A:507:GLN:CB	2.59	0.50
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.58	0.50
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.47	0.50
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.92	0.50
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.46	0.50
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.45	0.50
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.46	0.50
2:B:175:ASN:N	2:B:176:PRO:CD	2.75	0.49
2:B:395:LYS:O	2:B:399:GLU:HG3	2.12	0.49
1:A:63:ILE:HD12	1:A:63:ILE:N	2.27	0.49
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.47	0.49
2:B:65:LYS:HE2	2:B:72:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.95	0.49
1:A:244:ILE:HB	1:A:310:LEU:HD12	1.93	0.49
1:A:94:ILE:HD13	1:A:94:ILE:N	2.18	0.49
1:A:218:ASP:HB2	1:A:221:HIS:CD2	2.47	0.49
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.13	0.49
2:B:239:TRP:CD1	2:B:239:TRP:N	2.79	0.49
2:B:424:LYS:HD2	2:B:425:LEU:CD1	2.41	0.49
1:A:311:LYS:O	1:A:312:GLU:C	2.55	0.49
1:A:465:LYS:CG	1:A:466:VAL:N	2.76	0.49
2:B:106:VAL:CG1	2:B:107:THR:N	2.75	0.49
1:A:405:TYR:O	2:B:331:LYS:HD3	2.13	0.49
2:B:158:ALA:C	2:B:160:PHE:H	2.21	0.49
2:B:379:SER:OG	2:B:387:PRO:HD3	2.13	0.49
1:A:498:ASP:HA	1:A:536:VAL:O	2.13	0.48
1:A:546:GLU:OE1	2:B:284:ARG:HG2	2.13	0.48
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.94	0.48
1:A:28:GLU:O	1:A:32:LYS:HG3	2.13	0.48
1:A:94:ILE:CD1	1:A:94:ILE:N	2.76	0.48
1:A:91:GLN:CD	1:A:93:GLY:H	2.20	0.48
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.13	0.48
2:B:239:TRP:CZ3	2:B:378:GLU:HG3	2.48	0.48
1:A:540:LYS:C	1:A:542:ILE:N	2.71	0.48
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.78	0.48
2:B:24:TRP:HH2	2:B:61:PHE:CD2	2.32	0.48
2:B:193:LEU:HD22	2:B:201:LYS:HE3	1.95	0.48
1:A:8:VAL:O	1:A:121:ASP:HB2	2.14	0.48
1:A:97:PRO:HD3	1:A:229:TRP:CD1	2.48	0.48
1:A:184:MET:HE3	1:A:184:MET:CA	2.43	0.48
2:B:396:GLU:O	2:B:400:THR:CG2	2.61	0.47
2:B:175:ASN:H	2:B:176:PRO:HD3	1.79	0.47
2:B:175:ASN:C	2:B:177:ASP:H	2.21	0.47
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.22	0.47
1:A:378:GLU:O	1:A:382:ILE:HG12	2.14	0.47
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.14	0.47
2:B:242:GLN:HA	2:B:242:GLN:OE1	2.14	0.47
1:A:355:ALA:O	1:A:357:MET:N	2.48	0.47
2:B:108:VAL:O	2:B:109:LEU:HD23	2.13	0.47
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.15	0.47
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.96	0.47
2:B:203:GLU:O	2:B:207:GLN:HG2	2.15	0.47
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:O	1:A:163:SER:C	2.56	0.47
1:A:337:TRP:CZ3	1:A:368:LEU:HD13	2.49	0.47
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.49	0.47
1:A:84:THR:HB	1:A:154:LYS:HD3	1.96	0.47
1:A:402:TRP:CD1	1:A:402:TRP:C	2.93	0.47
1:A:475:GLN:OE1	1:A:501:TYR:CE1	2.68	0.47
2:B:43:LYS:C	2:B:45:GLY:H	2.23	0.47
1:A:233:GLU:HG3	1:A:242:GLN:HG2	1.97	0.47
2:B:24:TRP:CH2	2:B:61:PHE:CD2	3.03	0.47
2:B:24:TRP:HZ3	2:B:403:THR:HG21	1.76	0.47
1:A:246:LEU:O	1:A:247:PRO:O	2.32	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.14	0.46
1:A:509:GLN:N	1:A:510:PRO:HD3	2.30	0.46
2:B:27:THR:O	2:B:28:GLU:C	2.56	0.46
2:B:108:VAL:CG2	2:B:188:TYR:CE1	2.97	0.46
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.96	0.46
1:A:179:VAL:HG12	3:A:999:HBQ:H103	1.96	0.46
1:A:542:ILE:HG23	2:B:283:LEU:HD23	1.98	0.46
2:B:49:LYS:HA	2:B:143:ARG:O	2.15	0.46
2:B:78:ARG:HD3	2:B:411:ILE:HG22	1.98	0.46
1:A:50:ILE:HD12	1:A:50:ILE:HA	1.83	0.46
1:A:94:ILE:HB	1:A:95:PRO:HD2	1.97	0.46
1:A:356:ARG:CG	1:A:356:ARG:NH1	2.79	0.46
2:B:115:TYR:CE1	2:B:156:SER:C	2.94	0.46
2:B:142:ILE:N	2:B:142:ILE:HD12	2.29	0.46
1:A:209:LEU:O	1:A:214:LEU:HB2	2.15	0.46
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.46	0.46
1:A:241:VAL:HG11	1:A:270:ILE:HD12	1.98	0.46
1:A:402:TRP:CG	1:A:403:THR:N	2.84	0.46
1:A:443:ASP:CB	1:A:548:VAL:CG1	2.93	0.46
2:B:165:THR:HG23	2:B:166:LYS:H	1.81	0.46
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.98	0.46
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.98	0.46
1:A:108:VAL:C	1:A:109:LEU:HD12	2.41	0.46
1:A:325:LEU:HD11	1:A:383:TRP:CG	2.51	0.46
1:A:545:ASN:HA	1:A:548:VAL:CG2	2.46	0.46
2:B:112:GLY:O	2:B:115:TYR:HD2	1.98	0.46
2:B:376:THR:HG22	2:B:386:THR:HG22	1.98	0.46
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.51	0.45
2:B:243:PRO:HG2	2:B:431:LYS:HB3	1.97	0.45
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HB3	1:A:216:THR:CG2	2.45	0.45
1:A:194:GLU:HB2	1:A:197:GLN:HG3	1.98	0.45
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.98	0.45
2:B:356:ARG:CB	2:B:367:GLN:HG2	2.46	0.45
1:A:23:GLN:HG2	1:A:131:THR:O	2.16	0.45
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.16	0.45
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.99	0.45
1:A:417:VAL:O	1:A:417:VAL:CG1	2.65	0.45
1:A:540:LYS:HB2	1:A:542:ILE:HD12	1.98	0.45
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.16	0.45
1:A:261:VAL:O	1:A:262:GLY:C	2.58	0.45
2:B:242:GLN:HB3	2:B:243:PRO:HD2	1.98	0.45
1:A:116:PHE:HZ	1:A:151:GLN:HB2	1.79	0.45
1:A:370:GLU:O	1:A:371:ALA:C	2.59	0.45
1:A:426:TRP:O	1:A:427:TYR:HB3	2.17	0.45
1:A:451:LYS:HB3	1:A:472:THR:H	1.81	0.45
1:A:502:ALA:O	1:A:503:LEU:C	2.60	0.45
2:B:109:LEU:N	2:B:187:LEU:O	2.49	0.45
2:B:118:VAL:O	2:B:148:VAL:HA	2.17	0.45
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.45
1:A:301:LEU:C	1:A:301:LEU:CD2	2.88	0.45
1:A:451:LYS:C	1:A:472:THR:H	2.24	0.45
1:A:540:LYS:HB3	1:A:542:ILE:CG1	2.47	0.45
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.98	0.45
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.52	0.45
1:A:55:PRO:HD2	1:A:56:TYR:CE2	2.52	0.45
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.98	0.45
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.47	0.45
1:A:544:GLY:CA	1:A:547:GLN:HG2	2.46	0.45
2:B:50:ILE:CG1	2:B:143:ARG:HB3	2.47	0.45
2:B:116:PHE:C	2:B:118:VAL:H	2.24	0.45
2:B:273:GLY:O	2:B:275:LYS:HG3	2.17	0.45
2:B:413:GLU:HA	2:B:413:GLU:OE2	2.17	0.45
1:A:253:THR:O	1:A:256:ASP:HB2	2.17	0.44
1:A:138:GLU:OE1	1:A:138:GLU:HA	2.17	0.44
1:A:216:THR:HG22	1:A:217:PRO:CD	2.48	0.44
1:A:408:ALA:HB3	2:B:393:ILE:HB	2.00	0.44
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.33	0.44
2:B:135:ILE:HD12	2:B:135:ILE:H	1.82	0.44
2:B:201:LYS:O	2:B:204:GLU:HB3	2.17	0.44
1:A:3:SER:OG	1:A:4:PRO:CD	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:O	1:A:85:GLN:HB3	2.17	0.44
1:A:210:LEU:C	1:A:212:TRP:N	2.74	0.44
2:B:132:ILE:HB	2:B:142:ILE:HB	1.99	0.44
1:A:181:TYR:C	1:A:181:TYR:CD2	2.91	0.44
2:B:176:PRO:C	2:B:178:ILE:H	2.25	0.44
1:A:124:PHE:O	1:A:127:TYR:HD2	2.00	0.44
1:A:136:ASN:ND2	1:A:138:GLU:HB2	2.33	0.44
1:A:266:TRP:CH2	1:A:270:ILE:HD11	2.53	0.44
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.53	0.44
1:A:488:ASP:OD2	1:A:488:ASP:N	2.50	0.44
1:A:220:LYS:O	1:A:221:HIS:ND1	2.51	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.16	0.44
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.99	0.44
2:B:358:ARG:HD3	2:B:358:ARG:HA	1.82	0.44
1:A:91:GLN:OE1	1:A:92:LEU:N	2.51	0.44
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.99	0.44
1:A:216:THR:HG22	1:A:217:PRO:HD2	2.00	0.44
1:A:320:ASP:OD2	1:A:320:ASP:C	2.60	0.44
1:A:543:GLY:HA3	2:B:284:ARG:HA	2.00	0.44
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.52	0.44
2:B:242:GLN:HB2	2:B:430:GLU:CD	2.43	0.44
1:A:188:TYR:CG	3:A:999:HBQ:H131	2.53	0.43
1:A:235:HIS:O	1:A:318:TYR:OH	2.31	0.43
2:B:208:HIS:O	2:B:211:ARG:HB2	2.18	0.43
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.47	0.43
1:A:301:LEU:O	1:A:304:ALA:HB3	2.18	0.43
1:A:38:CYS:O	1:A:47:ILE:HD11	2.18	0.43
1:A:385:LYS:NZ	1:A:385:LYS:HB3	2.34	0.43
2:B:169:GLU:N	2:B:170:PRO:HD2	2.32	0.43
2:B:239:TRP:HB3	2:B:350:LYS:CE	2.39	0.43
1:A:254:VAL:O	1:A:255:ASN:C	2.61	0.43
1:A:453:GLY:O	1:A:469:LEU:N	2.39	0.43
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.18	0.43
2:B:99:GLY:O	2:B:100:LEU:C	2.62	0.43
1:A:411:ILE:HG22	1:A:412:PRO:O	2.19	0.43
1:A:442:VAL:HG22	1:A:496:VAL:O	2.19	0.43
1:A:380:ILE:CG2	2:B:25:PRO:HB2	2.45	0.43
1:A:41:MET:SD	1:A:73:LYS:HE3	2.59	0.43
1:A:98:ALA:HB2	1:A:349:LEU:O	2.18	0.43
1:A:167:ILE:O	1:A:170:PRO:HD2	2.19	0.43
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:O	1:A:264:LEU:HD23	2.19	0.43
1:A:281:LYS:O	1:A:284:ARG:HG3	2.19	0.42
1:A:368:LEU:O	1:A:372:VAL:HG23	2.19	0.42
1:A:400:THR:O	1:A:404:GLU:HG2	2.18	0.42
2:B:233:GLU:OE2	2:B:233:GLU:CA	2.66	0.42
2:B:298:GLU:O	2:B:299:ALA:C	2.62	0.42
2:B:353:LYS:NZ	2:B:430:GLU:HB2	2.34	0.42
1:A:122:GLU:CD	1:A:122:GLU:N	2.77	0.42
1:A:34:LEU:HB3	1:A:132:ILE:HD12	2.00	0.42
1:A:180:ILE:CG1	1:A:189:VAL:HG13	2.46	0.42
1:A:266:TRP:HZ3	1:A:270:ILE:HD12	1.83	0.42
1:A:451:LYS:O	1:A:471:ASP:CA	2.67	0.42
2:B:106:VAL:HB	2:B:234:LEU:HB2	2.01	0.42
1:A:58:THR:CG2	1:A:76:ASP:O	2.65	0.42
1:A:163:SER:O	1:A:164:MET:C	2.61	0.42
1:A:399:GLU:O	1:A:403:THR:HG22	2.20	0.42
2:B:208:HIS:HD1	2:B:208:HIS:C	2.27	0.42
1:A:43:LYS:C	1:A:45:GLY:N	2.77	0.42
1:A:114:ALA:O	1:A:115:TYR:C	2.61	0.42
1:A:295:LEU:HD12	1:A:300:GLU:OE1	2.19	0.42
1:A:329:ILE:CG2	1:A:330:GLN:N	2.82	0.42
1:A:451:LYS:O	1:A:472:THR:N	2.50	0.42
2:B:77:PHE:O	2:B:78:ARG:C	2.61	0.42
2:B:85:GLN:O	2:B:154:LYS:HE3	2.20	0.42
1:A:109:LEU:O	1:A:111:VAL:HG13	2.19	0.42
2:B:113:ASP:O	2:B:114:ALA:C	2.62	0.42
1:A:317:VAL:HG21	1:A:347:LYS:HE2	2.01	0.42
1:A:426:TRP:HB3	1:A:526:ILE:HD13	2.00	0.42
1:A:457:TYR:CE1	1:A:463:ARG:HD2	2.55	0.42
1:A:543:GLY:CA	2:B:283:LEU:O	2.61	0.42
2:B:209:LEU:C	2:B:211:ARG:N	2.75	0.42
2:B:297:GLU:O	2:B:300:GLU:HB3	2.19	0.42
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.37	0.42
2:B:111:VAL:HG22	2:B:185:ASP:O	2.19	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.93	0.42
1:A:329:ILE:HD11	1:A:375:ILE:HD12	2.01	0.41
1:A:376:THR:O	1:A:380:ILE:HG12	2.20	0.41
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.55	0.41
2:B:202:ILE:O	2:B:205:LEU:N	2.53	0.41
1:A:213:GLY:O	1:A:214:LEU:HD23	2.19	0.41
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:NE2	1:A:281:LYS:HD2	2.35	0.41
1:A:402:TRP:O	1:A:404:GLU:N	2.53	0.41
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.20	0.41
2:B:242:GLN:HG2	2:B:351:THR:O	2.20	0.41
1:A:106:VAL:CG2	1:A:236:PRO:HB3	2.45	0.41
1:A:194:GLU:O	1:A:197:GLN:N	2.53	0.41
1:A:441:TYR:HD2	1:A:544:GLY:HA3	1.84	0.41
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.09	0.41
2:B:424:LYS:CD	2:B:425:LEU:HD12	2.47	0.41
1:A:105:SER:C	1:A:106:VAL:CG2	2.93	0.41
1:A:120:LEU:O	1:A:122:GLU:N	2.53	0.41
1:A:247:PRO:O	1:A:307:ARG:NH1	2.51	0.41
2:B:121:ASP:O	2:B:125:ARG:HG3	2.19	0.41
2:B:175:ASN:O	2:B:177:ASP:N	2.40	0.41
2:B:178:ILE:HG12	2:B:191:SER:HB3	2.01	0.41
2:B:265:ASN:O	2:B:268:SER:OG	2.33	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.65	0.41
1:A:266:TRP:CE3	1:A:266:TRP:C	2.99	0.41
2:B:97:PRO:C	2:B:99:GLY:N	2.78	0.41
2:B:97:PRO:HG2	2:B:100:LEU:HB2	2.02	0.41
2:B:134:SER:O	2:B:135:ILE:C	2.63	0.41
1:A:120:LEU:O	1:A:121:ASP:C	2.62	0.41
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.02	0.41
2:B:191:SER:CB	2:B:193:LEU:HD12	2.50	0.41
1:A:61:PHE:HB2	1:A:74:LEU:HB3	2.03	0.41
1:A:108:VAL:HG21	1:A:227:PHE:CE1	2.56	0.41
1:A:149:LEU:N	1:A:149:LEU:HD12	2.36	0.41
1:A:301:LEU:O	1:A:302:GLU:C	2.63	0.41
1:A:376:THR:HG23	1:A:386:THR:HG23	2.03	0.41
1:A:504:GLY:O	1:A:506:ILE:N	2.54	0.41
2:B:206:ARG:O	2:B:207:GLN:C	2.64	0.41
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.86	0.41
1:A:125:ARG:O	1:A:126:LYS:C	2.63	0.41
1:A:218:ASP:H	1:A:221:HIS:CD2	2.36	0.41
1:A:332:GLN:HE21	1:A:332:GLN:HB3	1.57	0.41
1:A:379:SER:C	1:A:381:VAL:N	2.73	0.41
1:A:540:LYS:CB	1:A:542:ILE:HD12	2.51	0.41
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.21	0.41
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.61	0.40
1:A:122:GLU:HA	1:A:125:ARG:NE	2.37	0.40
1:A:276:VAL:O	1:A:277:ARG:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.55	0.40
2:B:28:GLU:HA	2:B:135:ILE:HD11	2.02	0.40
2:B:106:VAL:HG12	2:B:107:THR:N	2.35	0.40
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.47	0.40
1:A:100:LEU:HD13	3:A:999:HBQ:C4	2.51	0.40
1:A:155:GLY:O	1:A:156:SER:C	2.63	0.40
1:A:266:TRP:CZ3	1:A:270:ILE:CD1	3.04	0.40
2:B:336:GLN:C	2:B:337:TRP:CD1	3.00	0.40
1:A:123:ASP:O	1:A:126:LYS:CE	2.62	0.40
1:A:542:ILE:O	1:A:545:ASN:HB3	2.21	0.40
1:A:253:THR:O	1:A:257:ILE:HG13	2.20	0.40
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.51	0.40
2:B:377:THR:O	2:B:381:VAL:HG23	2.21	0.40
1:A:158:ALA:O	1:A:159:ILE:C	2.64	0.40
1:A:221:HIS:O	1:A:223:LYS:NZ	2.45	0.40
2:B:24:TRP:CD1	2:B:24:TRP:N	2.84	0.40
2:B:125:ARG:O	2:B:126:LYS:C	2.63	0.40
2:B:393:ILE:HG12	2:B:394:GLN:N	2.36	0.40
2:B:424:LYS:HD3	2:B:424:LYS:C	2.47	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:36:GLU:OE2	2:B:318:TYR:OH[4_446]	2.10	0.10

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	532/547 (97%)	457 (86%)	55 (10%)	20 (4%)	2 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	394/426 (92%)	353 (90%)	34 (9%)	7 (2%)	6	25
All	All	926/973 (95%)	810 (88%)	89 (10%)	27 (3%)	3	15

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	356	ARG
2	B	175	ASN
2	B	176	PRO
1	A	121	ASP
1	A	247	PRO
1	A	361	HIS
1	A	505	ILE
2	B	98	ALA
2	B	356	ARG
1	A	158	ALA
1	A	170	PRO
1	A	195	ILE
1	A	403	THR
2	B	66	LYS
1	A	133	PRO
1	A	230	MET
2	B	236	PRO
1	A	159	ILE
1	A	345	PRO
1	A	44	GLU
1	A	139	THR
1	A	97	PRO
2	B	9	PRO
1	A	4	PRO
1	A	156	SER
1	A	312	GLU

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	480/488 (98%)	437 (91%)	43 (9%)	9	28
2	B	365/388 (94%)	341 (93%)	24 (7%)	15	43
All	All	845/876 (96%)	778 (92%)	67 (8%)	11	34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	46	LYS
1	A	48	SER
1	A	90	VAL
1	A	94	ILE
1	A	97	PRO
1	A	101	GLU
1	A	106	VAL
1	A	113	ASP
1	A	115	TYR
1	A	117	SER
1	A	122	GLU
1	A	123	ASP
1	A	138	GLU
1	A	151	GLN
1	A	159	ILE
1	A	184	MET
1	A	205	LEU
1	A	216	THR
1	A	241	VAL
1	A	244	ILE
1	A	308	GLU
1	A	310	LEU
1	A	317	VAL
1	A	332	GLN
1	A	340	GLN
1	A	345	PRO
1	A	349	LEU
1	A	357	MET
1	A	369	THR
1	A	379	SER
1	A	402	TRP
1	A	424	LYS
1	A	472	THR

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Mol	Chain	Res	Type
1	A	474	ASN
1	A	477	THR
1	A	488	ASP
1	A	516	GLU
1	A	517	LEU
1	A	529	GLU
1	A	533	LEU
1	A	540	LYS
2	B	8	VAL
2	B	24	TRP
2	B	40	GLU
2	B	66	LYS
2	B	67	ASP
2	B	68	SER
2	B	137	ASN
2	B	139	THR
2	B	164	MET
2	B	165	THR
2	B	176	PRO
2	B	187	LEU
2	B	205	LEU
2	B	236	PRO
2	B	283	LEU
2	B	290	THR
2	B	303	LEU
2	B	323	LYS
2	B	364	ASP
2	B	368	LEU
2	B	370	GLU
2	B	400	THR
2	B	423	VAL
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	147	ASN
1	A	161	GLN
1	A	174	GLN
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	207	GLN
1	A	221	HIS
1	A	222	GLN
1	A	235	HIS
1	A	255	ASN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	474	ASN
1	A	480	GLN
1	A	500	GLN
1	A	507	GLN
1	A	512	GLN
1	A	545	ASN
2	B	57	ASN
2	B	147	ASN
2	B	182	GLN
2	B	197	GLN
2	B	255	ASN
2	B	332	GLN
2	B	361	HIS
2	B	394	GLN
2	B	418	ASN
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	1.18	0	1,8,10	2.36	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	280	CSD	OD1-SG-CB	2.36	109.96	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	HBQ	A	999	-	21,21,21	1.94	6 (28%)	28,30,30	0.94	2 (7%)

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	HBQ	A	999	-	-	1/10/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	HBQ	C4-C3	4.74	1.45	1.40
3	A	999	HBQ	C3-N1	3.39	1.47	1.42
3	A	999	HBQ	C11-N1	3.01	1.41	1.37
3	A	999	HBQ	O3-C11	2.77	1.25	1.21
3	A	999	HBQ	C6-C5	2.25	1.42	1.38
3	A	999	HBQ	C2-C1	2.21	1.56	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	HBQ	O3-C11-N1	-2.20	120.40	123.99
3	A	999	HBQ	O2-C12-C13	-2.09	101.58	107.13

There are no chirality outliers.

All (1) torsion outliers are listed below:

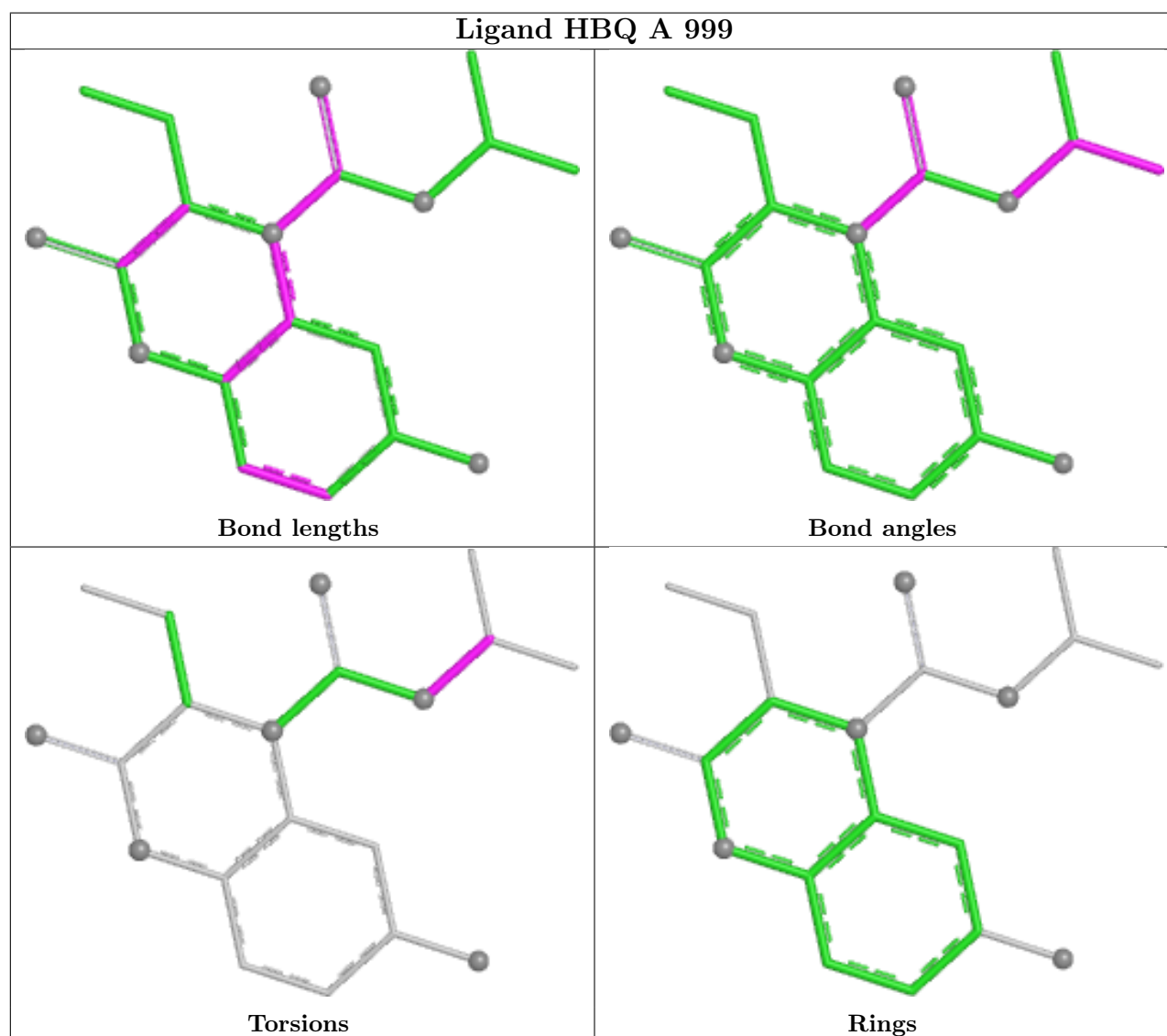
Mol	Chain	Res	Type	Atoms
3	A	999	HBQ	C13-C12-O2-C11

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	HBQ	5	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 ⓘ

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	538/547 (98%)	-0.36	1 (0%) 91 89	27, 90, 137, 150	0
2	B	400/426 (93%)	-0.40	0 100 100	48, 88, 139, 150	0
All	All	938/973 (96%)	-0.38	1 (0%) 92 90	27, 89, 139, 150	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	VAL	2.6

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	0.92	0.11	90,98,116,121	0

6.3 Carbohydrates [i](#)

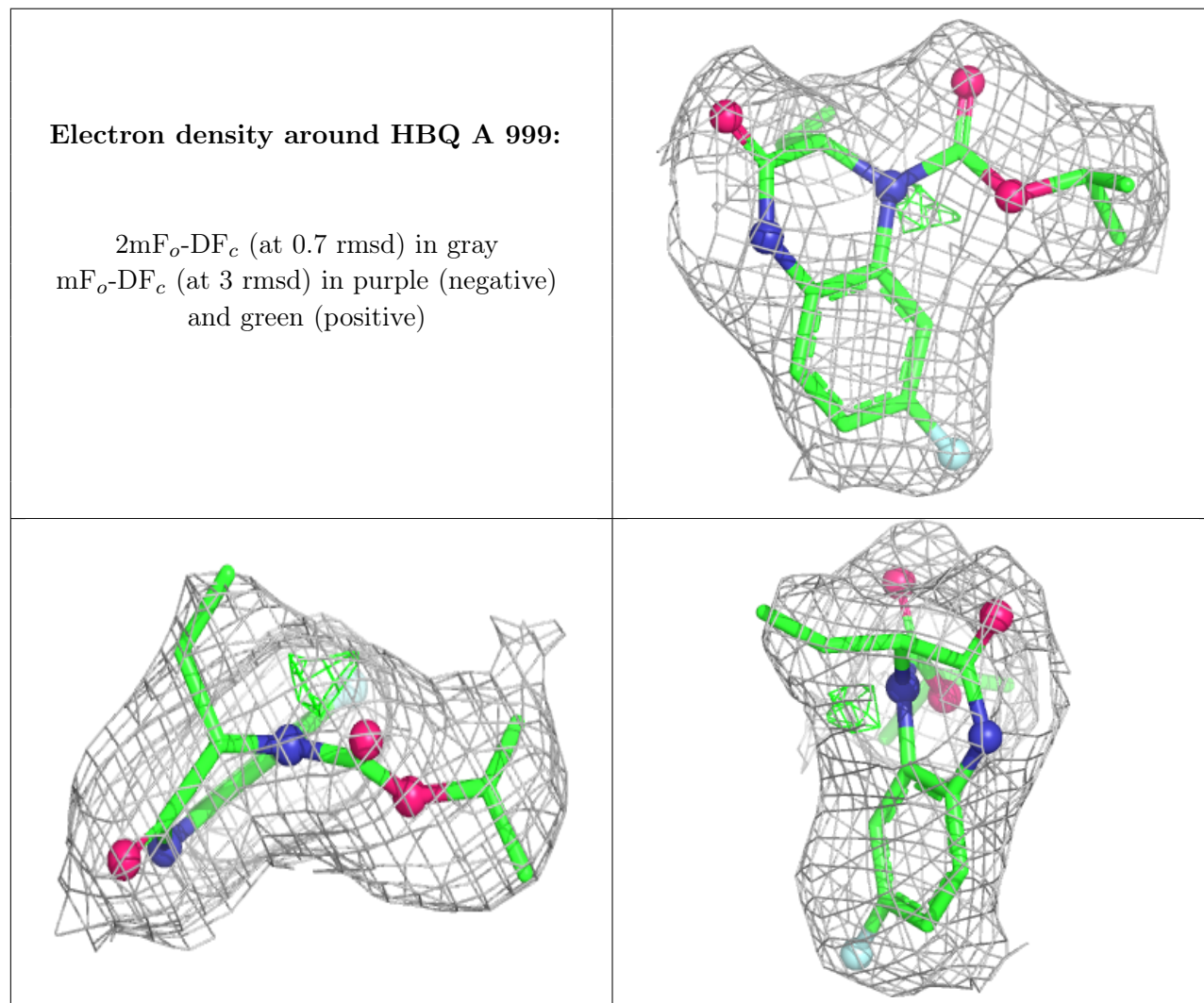
There are no oligosaccharides in this entry.

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	HBQ	A	999	20/20	0.96	0.08	47,61,70,87	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.