



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 AM UTC

PDB ID : 1DTT / pdb_00001dtt
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH PETT-2 (PETT130A94)
Authors : Ren, J.; Diprose, J.; Warren, J.; Esnouf, R.M.; Bird, L.E.; Ikemizu, S.; Slater, M.; Milton, J.; Balzarini, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2000-01-13
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

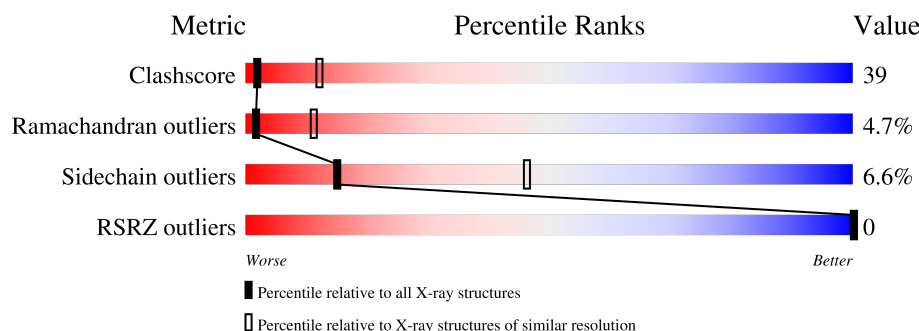
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

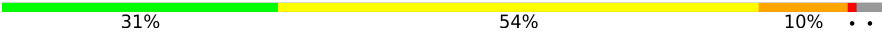
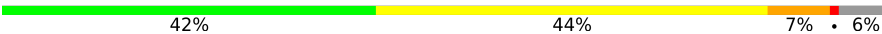
The reported resolution of this entry is 3.00 Å.

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))
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	
2	B	440	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSD	A	280	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7851 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.

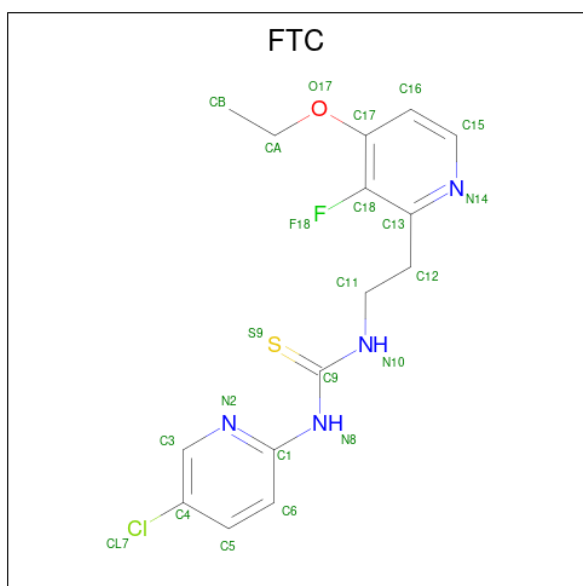
- Molecule 1 is a protein called HIV-1 RT A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4424	2862	737	817	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3404	2214	565	618	7			

- Molecule 3 is N-[[3-FLUORO-4-ETHOXY-PYRID-2-YL]ETHYL]-N'-[5-CHLORO-PYRIDYL]-THIOUREA (CCD ID: FTC) (formula: C₁₅H₁₆ClFN₄OS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			23	15	1	1	4	1	1		

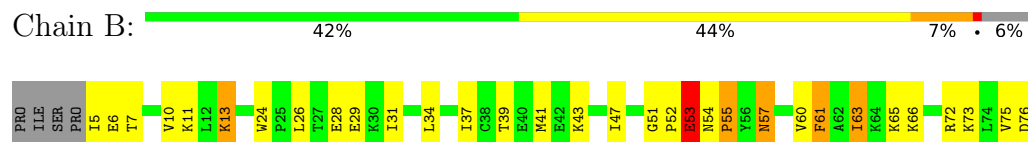
3 Residue-property plots

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	140.70Å 110.80Å 73.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.5 (30.00-3.00) 88.5 (30.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.276 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 100.5	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	0.96	EDS
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: FTC, 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	0.48	0/4530	0.98	15/6152 (0.2%)
2	B	0.47	0/3499	0.99	20/4752 (0.4%)
All	All	0.48	0/8029	0.98	35/10904 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	LYS	N-CA-C	-7.94	96.62	109.96
1	A	51	GLY	CA-C-N	6.76	128.29	119.84
1	A	51	GLY	C-N-CA	6.76	128.29	119.84
2	B	53	GLU	N-CA-C	-6.57	104.36	112.38
2	B	293	ILE	N-CA-C	6.41	115.23	107.61
1	A	184	MET	CB-CA-C	-6.35	109.27	116.63
2	B	428	GLN	N-CA-C	-6.28	104.49	111.71
2	B	13	LYS	N-CA-C	-6.24	101.71	109.64
2	B	349	LEU	N-CA-C	-6.16	105.90	113.41
2	B	118	VAL	N-CA-C	6.05	114.65	109.02
2	B	235	HIS	CA-C-N	6.01	125.72	119.82
2	B	235	HIS	C-N-CA	6.01	125.72	119.82
2	B	147	ASN	N-CA-C	-5.85	106.68	113.88
1	A	234	LEU	N-CA-C	5.73	118.81	109.59
2	B	83	ARG	N-CA-C	5.60	120.17	113.23
1	A	461	ARG	N-CA-C	-5.59	106.66	112.93
2	B	131	THR	N-CA-C	5.58	118.56	108.69
2	B	343	GLN	N-CA-C	-5.57	106.49	113.72
2	B	203	GLU	N-CA-C	-5.53	105.35	111.71
1	A	298	GLU	N-CA-C	-5.53	105.64	112.38
1	A	481	ALA	N-CA-C	-5.48	104.33	111.02
1	A	314	VAL	N-CA-C	5.46	115.72	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLY	CA-C-N	5.38	126.56	119.84
1	A	18	GLY	C-N-CA	5.38	126.56	119.84
2	B	101	LYS	N-CA-C	-5.36	105.34	111.07
1	A	493	VAL	N-CA-C	5.35	116.36	108.45
2	B	326	ILE	N-CA-C	5.33	117.00	108.89
2	B	391	LEU	N-CA-C	5.26	116.29	109.72
2	B	171	PHE	N-CA-C	-5.23	107.45	113.88
2	B	331	LYS	N-CA-C	-5.16	102.23	109.96
1	A	312	GLU	CA-C-N	5.14	126.27	119.84
1	A	312	GLU	C-N-CA	5.14	126.27	119.84
2	B	86	ASP	N-CA-C	-5.09	103.43	110.35
1	A	531	VAL	N-CA-C	5.03	115.36	108.12
2	B	57	ASN	N-CA-C	5.03	116.05	108.46

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	4424	0	4472	406	0
2	B	3404	0	3437	217	0
3	A	23	0	16	2	0
All	All	7851	0	7925	613	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 39.

All (613) 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:216:THR:HG22	1:A:217:PRO:HD2	1.37	1.07
1:A:65:LYS:HD2	1:A:72:ARG:HD3	1.37	1.06
1:A:274:ILE:HD11	1:A:310:LEU:HD11	1.34	1.05
2:B:98:ALA:HA	2:B:101:LYS:HD3	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.24	1.00
2:B:358:ARG:H	2:B:358:ARG:HD3	1.29	0.96
1:A:357:MET:HG2	1:A:358:ARG:H	1.30	0.95
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.29	0.95
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.47	0.94
1:A:228:LEU:H	1:A:228:LEU:HD23	1.33	0.94
1:A:23:GLN:HE22	1:A:60:VAL:H	1.14	0.93
2:B:5:ILE:HG22	2:B:6:GLU:H	1.34	0.90
2:B:424:LYS:HD3	2:B:425:LEU:N	1.87	0.88
2:B:98:ALA:CA	2:B:101:LYS:HD3	2.04	0.88
1:A:356:ARG:HH11	1:A:374:LYS:HZ2	1.18	0.87
1:A:41:MET:HB3	1:A:46:LYS:HE3	1.57	0.86
2:B:98:ALA:HA	2:B:101:LYS:CD	2.04	0.86
1:A:123:ASP:O	1:A:126:LYS:HD3	1.75	0.86
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.58	0.85
1:A:184:MET:HE3	1:A:184:MET:HA	1.58	0.85
2:B:422:LEU:HD12	2:B:422:LEU:H	1.43	0.83
1:A:65:LYS:HB3	1:A:72:ARG:NH1	1.94	0.83
1:A:245:VAL:HG13	1:A:307:ARG:HD2	1.61	0.82
1:A:361:HIS:CD2	1:A:510:PRO:HB3	2.15	0.81
1:A:57:ASN:HD22	1:A:58:THR:H	1.29	0.81
1:A:57:ASN:HD22	1:A:58:THR:N	1.78	0.81
1:A:356:ARG:HH11	1:A:374:LYS:NZ	1.77	0.81
2:B:88:TRP:HA	2:B:92:LEU:N	1.95	0.80
2:B:169:GLU:O	2:B:173:LYS:HG2	1.81	0.80
1:A:118:VAL:HB	1:A:149:LEU:HD13	1.62	0.80
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.16	0.80
1:A:47:ILE:HD12	1:A:47:ILE:H	1.47	0.80
1:A:441:TYR:HA	1:A:496:VAL:HG22	1.62	0.80
1:A:16:MET:HE3	1:A:83:ARG:HA	1.65	0.79
1:A:134:SER:C	1:A:135:ILE:HD12	2.08	0.79
1:A:173:LYS:O	1:A:176:PRO:HD3	1.83	0.79
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.64	0.79
1:A:516:GLU:O	1:A:520:GLN:HG2	1.82	0.79
1:A:75:VAL:HG12	1:A:76:ASP:H	1.48	0.78
1:A:122:GLU:H	1:A:122:GLU:CD	1.90	0.78
1:A:457:TYR:HE2	1:A:465:LYS:HD2	1.49	0.78
1:A:120:LEU:HD12	1:A:121:ASP:H	1.47	0.77
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.67	0.77
1:A:294:PRO:O	1:A:295:LEU:HB2	1.84	0.76
2:B:424:LYS:HD3	2:B:424:LYS:C	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG23	1:A:314:VAL:HB	1.68	0.76
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.16	0.76
1:A:260:LEU:HD21	1:A:303:LEU:HD21	1.67	0.75
1:A:356:ARG:NH1	1:A:374:LYS:HZ2	1.84	0.75
1:A:370:GLU:O	1:A:374:LYS:HG3	1.85	0.75
1:A:366:LYS:O	1:A:369:THR:HB	1.86	0.75
2:B:215:THR:HG22	2:B:217:PRO:HD3	1.69	0.75
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.68	0.75
2:B:119:PRO:HA	2:B:148:VAL:HA	1.67	0.75
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.23	0.74
2:B:66:LYS:HG3	2:B:407:GLN:NE2	2.03	0.73
1:A:499:SER:HB2	1:A:502:ALA:HB3	1.70	0.73
2:B:242:GLN:HB2	2:B:430:GLU:OE1	1.88	0.73
1:A:75:VAL:HG12	1:A:76:ASP:N	2.03	0.72
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.24	0.72
1:A:282:LEU:O	1:A:293:ILE:HD13	1.89	0.72
1:A:296:THR:O	1:A:299:ALA:HB3	1.88	0.72
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.72	0.72
1:A:132:ILE:HB	1:A:142:ILE:HG22	1.71	0.72
1:A:418:ASN:O	1:A:420:PRO:HD3	1.90	0.72
2:B:353:LYS:HB2	2:B:353:LYS:NZ	2.04	0.71
1:A:31:ILE:HG13	1:A:134:SER:O	1.90	0.71
1:A:125:ARG:HB3	1:A:146:TYR:O	1.89	0.71
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.70	0.71
2:B:163:SER:O	2:B:167:ILE:HG13	1.91	0.71
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.24	0.71
1:A:283:LEU:O	1:A:286:THR:HG23	1.91	0.70
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.71	0.70
1:A:489:SER:CB	1:A:493:VAL:HG21	2.21	0.70
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.26	0.70
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.26	0.70
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.74	0.70
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.73	0.70
1:A:48:SER:O	1:A:49:LYS:HB2	1.90	0.69
2:B:380:ILE:O	2:B:384:GLY:N	2.25	0.69
1:A:438:GLU:OE1	1:A:459:THR:HG21	1.91	0.69
2:B:51:GLY:HA3	2:B:53:GLU:OE2	1.92	0.69
2:B:296:THR:HG22	2:B:298:GLU:H	1.57	0.69
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.41	0.69
1:A:130:PHE:HB2	1:A:144:TYR:H	1.58	0.69
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.90	0.69
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.20	0.69
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.23	0.68
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.28	0.68
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.07	0.68
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.06	0.68
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.92	0.68
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.08	0.68
1:A:485:ALA:O	1:A:489:SER:HB3	1.94	0.68
1:A:506:ILE:HD12	1:A:506:ILE:H	1.57	0.68
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.75	0.68
2:B:115:TYR:HE1	2:B:157:PRO:HA	1.60	0.67
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.29	0.67
1:A:131:THR:HG22	1:A:133:PRO:HD3	1.75	0.67
1:A:161:GLN:HA	1:A:182:GLN:NE2	2.05	0.67
1:A:295:LEU:HD13	1:A:299:ALA:HB3	1.76	0.67
1:A:116:PHE:O	1:A:148:VAL:HG21	1.95	0.67
1:A:296:THR:HG22	1:A:298:GLU:OE2	1.94	0.67
2:B:11:LYS:O	2:B:85:GLN:HG2	1.94	0.67
1:A:57:ASN:ND2	1:A:58:THR:N	2.42	0.67
1:A:503:LEU:O	1:A:507:GLN:HB2	1.95	0.67
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.77	0.67
1:A:46:LYS:HB2	1:A:147:ASN:HD22	1.59	0.66
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.77	0.66
1:A:205:LEU:C	1:A:205:LEU:HD13	2.20	0.66
1:A:447:ASN:HB3	1:A:450:THR:HG23	1.78	0.66
2:B:263:LYS:HE2	2:B:425:LEU:HB3	1.78	0.66
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.77	0.66
1:A:451:LYS:HB3	1:A:472:THR:H	1.61	0.66
1:A:13:LYS:HB2	1:A:16:MET:HE2	1.76	0.66
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.77	0.65
1:A:243:PRO:HB3	1:A:313:PRO:HG3	1.79	0.65
1:A:516:GLU:OE1	1:A:516:GLU:HA	1.96	0.65
1:A:27:THR:O	1:A:31:ILE:HG12	1.94	0.65
1:A:274:ILE:CD1	1:A:310:LEU:HD11	2.21	0.65
2:B:209:LEU:HB3	2:B:214:LEU:HD21	1.78	0.65
1:A:210:LEU:CD1	1:A:215:THR:HA	2.26	0.65
1:A:295:LEU:HD12	1:A:300:GLU:HG3	1.78	0.65
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.25	0.65
1:A:279:LEU:C	1:A:281:LYS:N	2.55	0.65
1:A:111:VAL:HG12	1:A:216:THR:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:CSD:C	1:A:281:LYS:HA	2.27	0.64
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.79	0.64
1:A:210:LEU:HD13	1:A:215:THR:HA	1.80	0.64
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.32	0.64
1:A:506:ILE:HD12	1:A:506:ILE:N	2.12	0.64
1:A:396:GLU:O	1:A:400:THR:HG23	1.97	0.63
2:B:213:GLY:C	2:B:214:LEU:HD13	2.23	0.63
2:B:358:ARG:HD3	2:B:358:ARG:N	2.08	0.63
1:A:451:LYS:HB3	1:A:472:THR:N	2.13	0.63
2:B:72:ARG:HH21	2:B:151:GLN:NE2	1.97	0.63
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.29	0.63
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.47	0.63
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.80	0.62
1:A:244:ILE:HD13	1:A:263:LYS:HD3	1.82	0.62
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.64	0.62
2:B:241:VAL:HG22	2:B:242:GLN:N	2.15	0.62
2:B:194:GLU:HG2	2:B:195:ILE:N	2.14	0.62
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.81	0.61
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.81	0.61
1:A:92:LEU:C	1:A:92:LEU:HD22	2.26	0.61
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.00	0.61
1:A:65:LYS:HG3	1:A:68:SER:HB2	1.82	0.61
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.35	0.61
1:A:90:VAL:O	1:A:91:GLN:HB2	1.99	0.61
1:A:253:THR:O	1:A:256:ASP:HB2	2.00	0.61
1:A:542:ILE:HD12	1:A:542:ILE:H	1.65	0.60
1:A:506:ILE:H	1:A:506:ILE:CD1	2.14	0.60
1:A:47:ILE:HD12	1:A:47:ILE:N	2.16	0.60
1:A:47:ILE:H	1:A:47:ILE:CD1	2.14	0.60
1:A:122:GLU:HA	1:A:125:ARG:HE	1.65	0.60
2:B:72:ARG:NH2	2:B:151:GLN:HE22	2.00	0.60
1:A:64:LYS:HE3	1:A:71:TRP:CE3	2.37	0.60
2:B:422:LEU:HD12	2:B:422:LEU:N	2.16	0.60
1:A:17:ASP:O	1:A:83:ARG:HD3	2.01	0.60
1:A:441:TYR:HA	1:A:496:VAL:CG2	2.32	0.59
1:A:123:ASP:C	1:A:126:LYS:HD3	2.26	0.59
1:A:46:LYS:HD2	1:A:46:LYS:O	2.02	0.59
2:B:233:GLU:C	2:B:234:LEU:HD12	2.26	0.59
1:A:280:CSD:C	1:A:281:LYS:N	2.66	0.59
1:A:41:MET:HB3	1:A:46:LYS:CE	2.31	0.59
1:A:130:PHE:CD1	1:A:144:TYR:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:O	1:A:535:TRP:HA	2.03	0.58
2:B:63:ILE:HD13	2:B:63:ILE:H	1.69	0.58
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.02	0.58
2:B:233:GLU:O	2:B:234:LEU:HD12	2.03	0.58
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.86	0.58
1:A:242:GLN:HG2	1:A:242:GLN:O	2.04	0.58
2:B:120:LEU:HD23	2:B:121:ASP:N	2.19	0.58
2:B:353:LYS:HB2	2:B:353:LYS:HZ2	1.68	0.58
2:B:422:LEU:H	2:B:422:LEU:CD1	2.16	0.58
2:B:168:LEU:O	2:B:172:ARG:HG3	2.03	0.57
1:A:331:LYS:HG2	1:A:333:GLY:O	2.04	0.57
1:A:333:GLY:N	1:A:336:GLN:HG3	2.19	0.57
1:A:65:LYS:HB3	1:A:72:ARG:HH11	1.70	0.57
1:A:258:GLN:HE22	1:A:289:LEU:HD11	1.68	0.57
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.04	0.57
1:A:280:CSD:C	1:A:281:LYS:CA	2.83	0.57
1:A:365:VAL:HG11	1:A:401:TRP:CD2	2.40	0.57
1:A:64:LYS:HD3	1:A:69:THR:HA	1.85	0.57
1:A:120:LEU:HD12	1:A:121:ASP:N	2.19	0.57
1:A:125:ARG:HH11	1:A:147:ASN:HB3	1.67	0.57
1:A:301:LEU:HD23	1:A:301:LEU:O	2.04	0.57
1:A:295:LEU:CD1	1:A:300:GLU:HG3	2.35	0.56
2:B:5:ILE:HG22	2:B:6:GLU:N	2.13	0.56
2:B:65:LYS:NZ	2:B:72:ARG:NH1	2.52	0.56
2:B:210:LEU:HD11	2:B:216:THR:H	1.70	0.56
2:B:205:LEU:HD13	2:B:205:LEU:C	2.30	0.56
1:A:54:ASN:HD22	1:A:126:LYS:HB3	1.70	0.56
1:A:184:MET:HA	1:A:184:MET:CE	2.34	0.56
1:A:257:ILE:O	1:A:261:VAL:HG23	2.06	0.56
2:B:85:GLN:O	2:B:85:GLN:HG3	2.06	0.56
1:A:75:VAL:CG1	1:A:76:ASP:H	2.18	0.56
1:A:245:VAL:CG1	1:A:307:ARG:HD2	2.33	0.56
2:B:37:ILE:O	2:B:41:MET:HG3	2.05	0.56
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.88	0.56
1:A:517:LEU:O	1:A:520:GLN:HB2	2.06	0.56
1:A:542:ILE:HD12	1:A:542:ILE:N	2.20	0.56
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.87	0.56
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.05	0.56
2:B:374:LYS:O	2:B:377:THR:HB	2.05	0.56
1:A:56:TYR:O	1:A:129:ALA:HB3	2.05	0.56
1:A:77:PHE:O	1:A:78:ARG:C	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.41	0.56
1:A:249:LYS:HB3	1:A:252:TRP:CE2	2.41	0.56
2:B:200:THR:O	2:B:204:GLU:HB2	2.06	0.56
1:A:463:ARG:C	1:A:464:GLN:HG3	2.31	0.56
2:B:65:LYS:HZ2	2:B:72:ARG:HH11	1.52	0.56
2:B:380:ILE:O	2:B:384:GLY:CA	2.53	0.55
1:A:203:GLU:O	1:A:207:GLN:HG3	2.06	0.55
1:A:228:LEU:O	1:A:228:LEU:HG	2.06	0.55
1:A:340:GLN:HB2	1:A:351:THR:HG22	1.88	0.55
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.88	0.55
2:B:208:HIS:O	2:B:211:ARG:HB3	2.07	0.55
1:A:295:LEU:HD13	1:A:299:ALA:CB	2.37	0.55
2:B:356:ARG:HH12	2:B:358:ARG:HA	1.70	0.55
2:B:376:THR:O	2:B:380:ILE:HG12	2.06	0.55
1:A:358:ARG:HG2	1:A:512:GLN:HE21	1.72	0.55
1:A:228:LEU:H	1:A:228:LEU:CD2	2.10	0.55
1:A:64:LYS:HZ3	1:A:69:THR:HG22	1.72	0.55
2:B:214:LEU:O	2:B:215:THR:C	2.50	0.55
1:A:23:GLN:HE22	1:A:60:VAL:N	1.94	0.55
2:B:163:SER:HA	2:B:166:LYS:HE2	1.88	0.55
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.55	0.54
1:A:66:LYS:H	1:A:66:LYS:HD2	1.72	0.54
2:B:168:LEU:C	2:B:172:ARG:HG3	2.33	0.54
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.88	0.54
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.89	0.54
1:A:514:GLU:HG3	1:A:515:SER:N	2.22	0.54
2:B:92:LEU:N	2:B:92:LEU:HD23	2.22	0.54
1:A:94:ILE:HD12	1:A:94:ILE:N	2.22	0.54
2:B:97:PRO:O	2:B:98:ALA:HB2	2.08	0.54
2:B:276:VAL:HG22	2:B:276:VAL:O	2.07	0.54
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.90	0.54
1:A:23:GLN:NE2	1:A:60:VAL:H	1.94	0.54
1:A:118:VAL:O	1:A:148:VAL:HG23	2.07	0.54
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.23	0.54
1:A:329:ILE:HG22	1:A:330:GLN:N	2.22	0.53
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.72	0.53
1:A:495:ILE:O	1:A:533:LEU:HD23	2.08	0.53
1:A:57:ASN:N	1:A:143:ARG:HH22	2.05	0.53
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.68	0.53
1:A:122:GLU:HA	1:A:125:ARG:NE	2.24	0.53
2:B:98:ALA:C	2:B:101:LYS:HD3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.72	0.53
1:A:100:LEU:O	1:A:318:TYR:HB3	2.08	0.53
1:A:357:MET:HG2	1:A:358:ARG:N	2.12	0.53
1:A:243:PRO:CB	1:A:313:PRO:HG3	2.38	0.53
1:A:287:LYS:HG3	1:A:288:ALA:N	2.24	0.53
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.43	0.53
1:A:367:GLN:O	1:A:368:LEU:C	2.52	0.53
1:A:439:THR:O	1:A:459:THR:HA	2.09	0.53
2:B:253:THR:O	2:B:257:ILE:HG12	2.09	0.53
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.09	0.53
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.52
1:A:73:LYS:HD2	1:A:73:LYS:O	2.09	0.52
1:A:96:HIS:CD2	1:A:230:MET:HE1	2.44	0.52
1:A:394:GLN:HG2	1:A:396:GLU:OE2	2.08	0.52
2:B:175:ASN:C	2:B:177:ASP:H	2.17	0.52
2:B:61:PHE:N	2:B:61:PHE:CD2	2.78	0.52
1:A:235:HIS:HB2	1:A:238:LYS:O	2.09	0.52
2:B:120:LEU:HB2	2:B:148:VAL:O	2.09	0.52
2:B:425:LEU:O	2:B:429:LEU:HD13	2.10	0.52
1:A:118:VAL:O	1:A:148:VAL:CG2	2.57	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
1:A:474:ASN:CG	1:A:475:GLN:N	2.67	0.52
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.39	0.52
1:A:198:HIS:O	1:A:202:ILE:HG12	2.10	0.52
1:A:31:ILE:HD12	1:A:133:PRO:O	2.11	0.51
1:A:149:LEU:HD12	1:A:149:LEU:H	1.75	0.51
1:A:380:ILE:HD12	1:A:380:ILE:H	1.74	0.51
1:A:54:ASN:ND2	1:A:126:LYS:HB3	2.26	0.51
1:A:340:GLN:HA	1:A:351:THR:HA	1.93	0.51
2:B:332:GLN:OE1	2:B:424:LYS:HE3	2.09	0.51
1:A:507:GLN:C	1:A:509:GLN:H	2.18	0.51
1:A:523:GLU:HB3	1:A:527:LYS:NZ	2.25	0.51
1:A:27:THR:HG22	1:A:28:GLU:N	2.26	0.51
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.92	0.51
1:A:280:CSD:N	1:A:281:LYS:N	2.59	0.51
1:A:361:HIS:ND1	1:A:361:HIS:C	2.69	0.51
1:A:505:ILE:O	1:A:510:PRO:HD3	2.11	0.51
2:B:333:GLY:O	2:B:336:GLN:HB2	2.11	0.51
1:A:122:GLU:OE1	1:A:122:GLU:N	2.34	0.51
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.75	0.51
2:B:99:GLY:O	2:B:102:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASP:OD1	2:B:122:GLU:N	2.44	0.51
2:B:205:LEU:HD13	2:B:205:LEU:O	2.11	0.51
1:A:260:LEU:O	1:A:264:LEU:HD23	2.11	0.51
1:A:339:TYR:CD1	1:A:339:TYR:C	2.89	0.51
1:A:243:PRO:HG3	1:A:313:PRO:HG3	1.93	0.50
1:A:17:ASP:OD2	1:A:18:GLY:N	2.43	0.50
1:A:170:PRO:HG2	1:A:171:PHE:H	1.75	0.50
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.45	0.50
1:A:357:MET:CG	1:A:358:ARG:H	2.10	0.50
2:B:121:ASP:OD1	2:B:121:ASP:C	2.55	0.50
1:A:244:ILE:CD1	1:A:263:LYS:HD3	2.41	0.50
1:A:480:GLN:HE21	1:A:484:LEU:HG	1.76	0.50
2:B:332:GLN:NE2	2:B:424:LYS:HG2	2.27	0.50
2:B:267:ALA:CB	2:B:426:TRP:CH2	2.95	0.50
2:B:380:ILE:O	2:B:384:GLY:HA2	2.10	0.50
2:B:406:TRP:O	2:B:407:GLN:HG3	2.12	0.50
1:A:46:LYS:O	1:A:48:SER:N	2.44	0.50
2:B:115:TYR:CE1	2:B:157:PRO:HA	2.43	0.50
1:A:130:PHE:O	1:A:143:ARG:HG3	2.12	0.50
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.93	0.50
1:A:243:PRO:CG	1:A:313:PRO:HG3	2.42	0.49
1:A:441:TYR:CD2	1:A:496:VAL:HG21	2.47	0.49
2:B:65:LYS:HZ2	2:B:72:ARG:NH1	2.09	0.49
2:B:383:TRP:O	2:B:384:GLY:C	2.54	0.49
1:A:124:PHE:O	1:A:125:ARG:C	2.54	0.49
1:A:480:GLN:O	1:A:483:TYR:HB3	2.12	0.49
1:A:109:LEU:HD12	1:A:109:LEU:N	2.27	0.49
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.26	0.49
1:A:310:LEU:N	1:A:310:LEU:HD12	2.28	0.49
1:A:179:VAL:HG11	3:A:999:FTC:H112	1.93	0.49
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.94	0.49
2:B:244:ILE:HG13	2:B:426:TRP:HZ2	1.75	0.49
1:A:309:ILE:C	1:A:311:LYS:H	2.21	0.49
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.43	0.49
2:B:39:THR:O	2:B:43:LYS:HG2	2.12	0.49
2:B:116:PHE:O	2:B:117:SER:C	2.54	0.49
1:A:474:ASN:OD1	1:A:475:GLN:HG3	2.13	0.49
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.48	0.49
2:B:101:LYS:HG2	2:B:382:ILE:HA	1.95	0.49
2:B:334:GLN:C	2:B:336:GLN:H	2.21	0.49
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.94	0.48
2:B:424:LYS:HD3	2:B:425:LEU:CA	2.42	0.48
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.94	0.48
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.42	0.48
1:A:13:LYS:HE3	1:A:84:THR:O	2.13	0.48
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.46	0.48
2:B:191:SER:OG	2:B:198:HIS:ND1	2.40	0.48
2:B:393:ILE:O	2:B:416:PHE:HB3	2.13	0.48
1:A:324:ASP:O	1:A:343:GLN:HG2	2.14	0.48
1:A:474:ASN:O	1:A:478:GLU:HG3	2.13	0.48
1:A:241:VAL:O	1:A:243:PRO:HD3	2.14	0.48
1:A:320:ASP:OD1	1:A:323:LYS:HG2	2.14	0.48
1:A:442:VAL:HG22	1:A:496:VAL:O	2.13	0.48
1:A:427:TYR:CE2	1:A:509:GLN:HG3	2.49	0.48
2:B:52:PRO:C	2:B:54:ASN:N	2.69	0.48
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.47	0.48
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.96	0.48
1:A:245:VAL:HG13	1:A:307:ARG:CD	2.38	0.48
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.42	0.48
2:B:28:GLU:O	2:B:31:ILE:N	2.46	0.48
1:A:312:GLU:O	1:A:312:GLU:HG3	2.13	0.48
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.49	0.48
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.49	0.48
1:A:457:TYR:CE2	1:A:465:LYS:HD2	2.38	0.48
1:A:470:THR:O	1:A:471:ASP:HB3	2.13	0.48
1:A:87:PHE:N	1:A:87:PHE:CD1	2.82	0.47
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.96	0.47
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.14	0.47
1:A:24:TRP:H	1:A:24:TRP:CD1	2.32	0.47
1:A:311:LYS:O	1:A:313:PRO:HD3	2.14	0.47
1:A:36:GLU:O	1:A:36:GLU:HG2	2.13	0.47
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.97	0.47
1:A:472:THR:OG1	1:A:473:THR:N	2.47	0.47
2:B:10:VAL:HG12	2:B:11:LYS:N	2.29	0.47
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.79	0.47
1:A:66:LYS:HD2	1:A:66:LYS:N	2.30	0.47
1:A:345:PRO:O	1:A:346:PHE:HB2	2.15	0.47
2:B:278:GLN:HA	2:B:278:GLN:NE2	2.29	0.47
2:B:296:THR:HG22	2:B:298:GLU:N	2.26	0.47
1:A:4:PRO:HG2	1:A:212:TRP:CZ3	2.49	0.47
1:A:130:PHE:O	1:A:143:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:O	1:A:259:LYS:HG3	2.15	0.47
1:A:282:LEU:H	1:A:282:LEU:HD22	1.79	0.47
1:A:359:GLY:C	1:A:361:HIS:H	2.21	0.47
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.13	0.47
1:A:520:GLN:OE1	1:A:520:GLN:HA	2.14	0.47
2:B:318:TYR:HE1	2:B:320:ASP:HB2	1.80	0.47
1:A:452:LEU:HD12	1:A:469:LEU:O	2.14	0.47
1:A:491:LEU:O	1:A:529:GLU:HB3	2.15	0.47
2:B:231:GLY:O	2:B:232:TYR:HB2	2.15	0.47
1:A:8:VAL:HG21	1:A:159:ILE:HG12	1.97	0.47
1:A:137:ASN:O	1:A:138:GLU:HB3	2.15	0.47
1:A:240:THR:HA	1:A:314:VAL:O	2.15	0.47
1:A:506:ILE:N	1:A:506:ILE:CD1	2.77	0.47
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.47
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.44	0.47
1:A:51:GLY:O	1:A:53:GLU:N	2.48	0.47
1:A:125:ARG:O	1:A:128:THR:OG1	2.28	0.47
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.15	0.47
2:B:209:LEU:O	2:B:210:LEU:C	2.58	0.47
1:A:149:LEU:HD12	1:A:149:LEU:N	2.30	0.46
1:A:149:LEU:H	1:A:149:LEU:CD1	2.28	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.44	0.46
1:A:451:LYS:O	1:A:471:ASP:N	2.45	0.46
1:A:345:PRO:C	1:A:346:PHE:HD1	2.23	0.46
2:B:63:ILE:HD13	2:B:63:ILE:N	2.30	0.46
2:B:120:LEU:HD21	2:B:124:PHE:HB3	1.97	0.46
1:A:450:THR:O	1:A:452:LEU:N	2.48	0.46
1:A:477:THR:O	1:A:480:GLN:HB3	2.15	0.46
2:B:7:THR:HG23	2:B:7:THR:O	2.15	0.46
2:B:376:THR:CG2	2:B:386:THR:HG22	2.45	0.46
1:A:12:LEU:O	1:A:13:LYS:C	2.57	0.46
1:A:101:LYS:O	3:A:999:FTC:H6	2.16	0.46
1:A:219:LYS:HA	1:A:222:GLN:CD	2.40	0.46
1:A:226:PRO:HA	1:A:234:LEU:O	2.15	0.46
1:A:505:ILE:O	1:A:510:PRO:CD	2.64	0.46
2:B:125:ARG:NE	2:B:147:ASN:HA	2.31	0.46
1:A:317:VAL:O	1:A:349:LEU:HD23	2.15	0.46
2:B:317:VAL:HG23	2:B:317:VAL:O	2.16	0.46
1:A:92:LEU:HD21	2:B:137:ASN:OD1	2.16	0.46
1:A:337:TRP:O	1:A:353:LYS:HA	2.15	0.46
1:A:507:GLN:O	1:A:509:GLN:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:PRO:HD2	2:B:53:GLU:OE2	2.16	0.46
2:B:63:ILE:O	2:B:72:ARG:HB3	2.16	0.46
2:B:155:GLY:O	2:B:158:ALA:HB3	2.15	0.46
2:B:353:LYS:HB2	2:B:353:LYS:HZ3	1.81	0.46
2:B:371:ALA:O	2:B:372:VAL:C	2.59	0.46
1:A:171:PHE:CD1	1:A:205:LEU:HD23	2.51	0.46
2:B:209:LEU:C	2:B:211:ARG:N	2.70	0.46
1:A:31:ILE:HG21	1:A:134:SER:HA	1.97	0.46
1:A:241:VAL:HG11	1:A:270:ILE:HD13	1.98	0.46
1:A:320:ASP:OD2	1:A:322:SER:HB3	2.15	0.46
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.99	0.46
2:B:168:LEU:O	2:B:169:GLU:C	2.59	0.46
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.51	0.46
1:A:12:LEU:HD12	1:A:83:ARG:O	2.16	0.45
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.50	0.45
2:B:28:GLU:O	2:B:29:GLU:C	2.57	0.45
2:B:165:THR:OG1	2:B:166:LYS:N	2.49	0.45
2:B:194:GLU:HG2	2:B:196:GLY:H	1.81	0.45
1:A:64:LYS:NZ	1:A:69:THR:HG22	2.30	0.45
1:A:92:LEU:HD13	1:A:93:GLY:N	2.31	0.45
1:A:118:VAL:HB	1:A:149:LEU:CD1	2.40	0.45
1:A:229:TRP:CG	1:A:230:MET:H	2.33	0.45
1:A:301:LEU:O	1:A:305:GLU:HB2	2.16	0.45
2:B:78:ARG:HD3	2:B:411:ILE:O	2.17	0.45
1:A:120:LEU:CD1	1:A:121:ASP:H	2.24	0.45
1:A:162:SER:O	1:A:165:THR:HB	2.16	0.45
2:B:121:ASP:OD1	2:B:123:ASP:N	2.48	0.45
2:B:194:GLU:C	2:B:196:GLY:H	2.25	0.45
1:A:77:PHE:O	1:A:80:LEU:N	2.49	0.45
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.98	0.45
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.98	0.45
2:B:158:ALA:O	2:B:161:GLN:HB2	2.16	0.45
2:B:206:ARG:HG3	2:B:216:THR:O	2.17	0.45
2:B:267:ALA:C	2:B:269:GLN:H	2.24	0.45
1:A:46:LYS:HD2	1:A:48:SER:HB3	1.98	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.45
1:A:399:GLU:O	1:A:403:THR:HG23	2.17	0.45
1:A:361:HIS:NE2	1:A:508:ALA:HB1	2.32	0.45
1:A:377:THR:O	1:A:378:GLU:C	2.59	0.45
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.45	0.45
1:A:474:ASN:O	1:A:477:THR:OG1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ASN:O	2:B:259:LYS:HG3	2.17	0.45
2:B:339:TYR:C	2:B:340:GLN:NE2	2.75	0.45
1:A:7:THR:HG22	1:A:119:PRO:O	2.17	0.45
1:A:419:THR:HG23	1:A:419:THR:O	2.17	0.45
1:A:506:ILE:O	1:A:507:GLN:C	2.60	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.45
1:A:171:PHE:CG	1:A:205:LEU:HD23	2.52	0.45
1:A:505:ILE:HG22	1:A:506:ILE:HD12	1.99	0.45
1:A:129:ALA:HB1	1:A:143:ARG:CZ	2.47	0.44
1:A:379:SER:O	1:A:380:ILE:C	2.60	0.44
2:B:79:GLU:O	2:B:83:ARG:HG3	2.17	0.44
1:A:49:LYS:HA	1:A:144:TYR:HA	1.98	0.44
1:A:88:TRP:O	1:A:89:GLU:C	2.59	0.44
1:A:157:PRO:O	1:A:158:ALA:C	2.59	0.44
1:A:514:GLU:HG3	1:A:515:SER:H	1.82	0.44
2:B:241:VAL:HG22	2:B:242:GLN:H	1.81	0.44
1:A:229:TRP:O	1:A:231:GLY:N	2.48	0.44
1:A:317:VAL:HG22	1:A:318:TYR:N	2.32	0.44
1:A:253:THR:OG1	1:A:256:ASP:CG	2.59	0.44
1:A:342:TYR:CD1	1:A:342:TYR:C	2.95	0.44
2:B:100:LEU:HA	2:B:103:LYS:HB2	2.00	0.44
2:B:426:TRP:O	2:B:429:LEU:HB2	2.17	0.44
1:A:47:ILE:HG22	1:A:47:ILE:O	2.16	0.44
1:A:250:ASP:CG	1:A:251:SER:N	2.75	0.44
1:A:329:ILE:HD12	1:A:391:LEU:HD22	2.00	0.44
1:A:339:TYR:C	1:A:340:GLN:NE2	2.75	0.44
1:A:542:ILE:H	1:A:542:ILE:CD1	2.31	0.44
2:B:193:LEU:N	2:B:193:LEU:HD22	2.33	0.44
2:B:367:GLN:O	2:B:368:LEU:C	2.59	0.44
1:A:126:LYS:H	1:A:126:LYS:HG3	1.57	0.44
2:B:126:LYS:HG3	2:B:127:TYR:N	2.32	0.44
2:B:203:GLU:O	2:B:207:GLN:HG3	2.17	0.44
1:A:171:PHE:CE1	1:A:205:LEU:HB2	2.51	0.44
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.48	0.44
2:B:374:LYS:O	2:B:378:GLU:HG3	2.17	0.44
1:A:95:PRO:HG3	2:B:137:ASN:O	2.17	0.44
1:A:216:THR:HG22	1:A:217:PRO:CD	2.26	0.44
1:A:344:GLU:HB2	1:A:347:LYS:HB2	2.00	0.44
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.99	0.44
1:A:451:LYS:HD2	1:A:472:THR:O	2.17	0.43
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:CB	1:A:471:ASP:HA	2.48	0.43
2:B:370:GLU:O	2:B:371:ALA:C	2.62	0.43
1:A:64:LYS:HG3	1:A:71:TRP:CE2	2.53	0.43
1:A:126:LYS:C	1:A:128:THR:H	2.25	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.33	0.43
1:A:230:MET:O	1:A:232:TYR:CD1	2.72	0.43
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.99	0.43
1:A:458:VAL:HA	1:A:463:ARG:O	2.18	0.43
2:B:268:SER:HA	2:B:271:TYR:O	2.18	0.43
1:A:46:LYS:NZ	1:A:48:SER:OG	2.50	0.43
2:B:13:LYS:HE2	2:B:86:ASP:OD2	2.19	0.43
2:B:77:PHE:O	2:B:78:ARG:C	2.59	0.43
2:B:115:TYR:HE2	2:B:185:ASP:HA	1.82	0.43
2:B:206:ARG:O	2:B:210:LEU:HD13	2.18	0.43
1:A:66:LYS:O	1:A:67:ASP:HB2	2.19	0.43
1:A:282:LEU:HD22	1:A:282:LEU:N	2.34	0.43
1:A:435:VAL:HA	2:B:290:THR:HG21	2.00	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.80	0.43
1:A:270:ILE:HG22	1:A:314:VAL:HG21	2.01	0.43
1:A:409:THR:O	2:B:364:ASP:HB2	2.18	0.43
2:B:194:GLU:C	2:B:196:GLY:N	2.76	0.43
1:A:184:MET:HB3	1:A:185:ASP:H	1.50	0.43
2:B:369:THR:O	2:B:370:GLU:C	2.62	0.43
2:B:75:VAL:HG12	2:B:76:ASP:N	2.33	0.43
2:B:87:PHE:CD1	2:B:87:PHE:N	2.87	0.43
1:A:91:GLN:C	1:A:93:GLY:H	2.26	0.43
1:A:110:ASP:C	1:A:112:GLY:H	2.26	0.43
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.81	0.43
2:B:214:LEU:HD13	2:B:214:LEU:N	2.34	0.43
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.49	0.42
1:A:359:GLY:C	1:A:361:HIS:N	2.76	0.42
1:A:19:PRO:HG3	1:A:83:ARG:HD2	2.00	0.42
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.34	0.42
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.91	0.42
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.01	0.42
1:A:194:GLU:O	1:A:195:ILE:C	2.61	0.42
1:A:205:LEU:C	1:A:205:LEU:CD1	2.92	0.42
2:B:195:ILE:HG12	2:B:195:ILE:O	2.19	0.42
1:A:7:THR:HG21	1:A:120:LEU:O	2.19	0.42
2:B:245:VAL:O	2:B:245:VAL:HG13	2.19	0.42
1:A:27:THR:HG22	1:A:28:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG23	1:A:111:VAL:O	2.18	0.42
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.91	0.42
1:A:366:LYS:HD3	1:A:405:TYR:OH	2.19	0.42
2:B:173:LYS:O	2:B:176:PRO:HD3	2.20	0.42
2:B:241:VAL:CG2	2:B:242:GLN:N	2.81	0.42
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.42
1:A:258:GLN:HE22	1:A:289:LEU:CD1	2.33	0.42
2:B:345:PRO:O	2:B:346:PHE:HB2	2.20	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:480:GLN:NE2	1:A:483:TYR:HD2	2.11	0.42
2:B:358:ARG:H	2:B:358:ARG:CD	2.10	0.42
1:A:447:ASN:C	1:A:447:ASN:HD22	2.27	0.42
1:A:452:LEU:HA	1:A:469:LEU:O	2.20	0.42
1:A:508:ALA:O	1:A:509:GLN:C	2.62	0.42
2:B:180:ILE:HA	2:B:188:TYR:O	2.19	0.42
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.42
1:A:478:GLU:HB3	1:A:499:SER:OG	2.20	0.42
2:B:201:LYS:HE2	2:B:204:GLU:OE2	2.19	0.42
2:B:326:ILE:CG2	2:B:327:ALA:N	2.82	0.42
1:A:309:ILE:O	1:A:311:LYS:N	2.53	0.42
1:A:390:LYS:HE2	1:A:415:GLU:OE2	2.20	0.42
1:A:486:LEU:HA	1:A:528:LYS:HE3	2.02	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.42
1:A:91:GLN:C	1:A:93:GLY:N	2.74	0.41
1:A:489:SER:OG	1:A:493:VAL:HG21	2.19	0.41
1:A:477:THR:O	1:A:478:GLU:C	2.62	0.41
1:A:46:LYS:C	1:A:147:ASN:ND2	2.78	0.41
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.35	0.41
1:A:241:VAL:O	1:A:243:PRO:CD	2.69	0.41
2:B:97:PRO:HG2	2:B:100:LEU:CD2	2.50	0.41
1:A:285:GLY:O	1:A:286:THR:C	2.64	0.41
1:A:418:ASN:C	1:A:420:PRO:HD3	2.44	0.41
1:A:537:PRO:HG3	2:B:262:GLY:HA2	2.03	0.41
2:B:79:GLU:O	2:B:82:LYS:HB2	2.20	0.41
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.41
1:A:105:SER:O	1:A:190:GLY:HA2	2.21	0.41
1:A:129:ALA:CB	1:A:143:ARG:NH2	2.83	0.41
1:A:253:THR:HG22	1:A:292:VAL:HG22	2.03	0.41
2:B:34:LEU:HD21	2:B:73:LYS:HG3	2.02	0.41
2:B:120:LEU:HD12	2:B:150:PRO:HD3	2.01	0.41
1:A:412:PRO:O	1:A:413:GLU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:O	1:A:482:ILE:HB	2.20	0.41
1:A:522:ILE:O	1:A:526:ILE:HG13	2.20	0.41
2:B:380:ILE:HA	2:B:384:GLY:HA2	2.01	0.41
1:A:358:ARG:CD	1:A:512:GLN:HE21	2.33	0.41
1:A:451:LYS:O	1:A:471:ASP:HA	2.21	0.41
2:B:100:LEU:N	2:B:100:LEU:HD23	2.36	0.41
1:A:97:PRO:HD3	1:A:230:MET:HE2	2.02	0.41
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.02	0.41
1:A:363:ASN:OD1	1:A:365:VAL:HB	2.20	0.41
2:B:164:MET:HE2	2:B:168:LEU:HD11	2.03	0.41
2:B:193:LEU:HD22	2:B:193:LEU:H	1.86	0.41
2:B:206:ARG:NH1	2:B:206:ARG:HG2	2.36	0.41
1:A:92:LEU:HD22	1:A:92:LEU:O	2.20	0.41
2:B:175:ASN:CG	2:B:201:LYS:HZ1	2.29	0.41
2:B:252:TRP:HB3	2:B:257:ILE:HD11	2.02	0.41
1:A:27:THR:HG22	1:A:29:GLU:H	1.86	0.40
1:A:160:PHE:O	1:A:161:GLN:C	2.64	0.40
1:A:358:ARG:HB2	1:A:358:ARG:CZ	2.51	0.40
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.97	0.40
1:A:35:VAL:HG12	1:A:36:GLU:N	2.35	0.40
1:A:170:PRO:O	1:A:171:PHE:C	2.64	0.40
2:B:175:ASN:ND2	2:B:201:LYS:HZ3	2.18	0.40
2:B:360:ALA:CB	2:B:366:LYS:HD3	2.43	0.40
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.21	0.40
1:A:291:GLU:HG2	1:A:292:VAL:N	2.36	0.40
2:B:53:GLU:O	2:B:55:PRO:HD3	2.21	0.40
1:A:46:LYS:CB	1:A:147:ASN:HD22	2.33	0.40
1:A:118:VAL:CG1	1:A:119:PRO:HD2	2.50	0.40
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.03	0.40
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.51	0.40
1:A:345:PRO:C	1:A:346:PHE:CD1	3.00	0.40
1:A:77:PHE:O	1:A:79:GLU:N	2.55	0.40
1:A:275:LYS:C	1:A:276:VAL:HG13	2.47	0.40
2:B:78:ARG:O	2:B:82:LYS:HG3	2.22	0.40
2:B:98:ALA:O	2:B:101:LYS:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	535/560 (96%)	422 (79%)	79 (15%)	34 (6%)	1	6
2	B	406/440 (92%)	338 (83%)	58 (14%)	10 (2%)	4	23
All	All	941/1000 (94%)	760 (81%)	137 (15%)	44 (5%)	2	11

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
1	A	47	ILE
1	A	49	LYS
1	A	67	ASP
1	A	73	LYS
1	A	134	SER
1	A	294	PRO
1	A	295	LEU
1	A	451	LYS
1	A	487	GLN
1	A	505	ILE
1	A	538	ALA
2	B	97	PRO
2	B	98	ALA
2	B	232	TYR
1	A	52	PRO
1	A	66	LYS
1	A	85	GLN
1	A	112	GLY
1	A	195	ILE
1	A	310	LEU
1	A	313	PRO
1	A	508	ALA
1	A	540	LYS
2	B	215	THR

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Mol	Chain	Res	Type
2	B	358	ARG
1	A	45	GLY
1	A	78	ARG
1	A	131	THR
1	A	136	ASN
1	A	539	HIS
2	B	214	LEU
2	B	241	VAL
2	B	356	ARG
1	A	91	GLN
1	A	113	ASP
1	A	127	TYR
1	A	242	GLN
1	A	276	VAL
1	A	111	VAL
2	B	431	LYS
1	A	25	PRO
1	A	170	PRO
2	B	176	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/499 (97%)	450 (93%)	34 (7%)	14	44
2	B	374/400 (94%)	351 (94%)	23 (6%)	17	49
All	All	858/899 (95%)	801 (93%)	57 (7%)	15	46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	29	GLU
1	A	36	GLU
1	A	71	TRP

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	88	TRP
1	A	92	LEU
1	A	108	VAL
1	A	122	GLU
1	A	150	PRO
1	A	173	LYS
1	A	184	MET
1	A	197	GLN
1	A	216	THR
1	A	240	THR
1	A	263	LYS
1	A	264	LEU
1	A	274	ILE
1	A	289	LEU
1	A	295	LEU
1	A	330	GLN
1	A	332	GLN
1	A	340	GLN
1	A	347	LYS
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	386	THR
1	A	394	GLN
1	A	423	VAL
1	A	458	VAL
1	A	465	LYS
1	A	488	ASP
1	A	533	LEU
2	B	24	TRP
2	B	53	GLU
2	B	55	PRO
2	B	60	VAL
2	B	61	PHE
2	B	63	ILE
2	B	88	TRP
2	B	92	LEU
2	B	139	THR
2	B	184	MET
2	B	214	LEU
2	B	246	LEU

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Mol	Chain	Res	Type
2	B	283	LEU
2	B	289	LEU
2	B	336	GLN
2	B	353	LYS
2	B	358	ARG
2	B	368	LEU
2	B	422	LEU
2	B	423	VAL
2	B	424	LYS
2	B	425	LEU
2	B	431	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	137	ASN
1	A	145	GLN
1	A	147	ASN
1	A	174	GLN
1	A	175	ASN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	208	HIS
1	A	255	ASN
1	A	258	GLN
1	A	332	GLN
1	A	340	GLN
1	A	394	GLN
1	A	407	GLN
1	A	428	GLN
1	A	447	ASN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	512	GLN
1	A	519	ASN
2	B	57	ASN
2	B	85	GLN
2	B	147	ASN

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Mol	Chain	Res	Type
2	B	151	GLN
2	B	174	GLN
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	348	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	1.55	1 (25%)	1,8,10	4.24	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	2.85	1.50	1.47

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	4.24	113.41	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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	4	0

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	FTC	A	999	-	24,24,24	1.66	6 (25%)	29,31,31	2.29	11 (37%)

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	FTC	A	999	-	-	5/13/13/13	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	FTC	C13-N14	3.21	1.38	1.34
3	A	999	FTC	C1-N2	3.20	1.40	1.34
3	A	999	FTC	C9-S9	2.83	1.74	1.68
3	A	999	FTC	C3-N2	2.59	1.39	1.34
3	A	999	FTC	C17-C18	2.45	1.42	1.39
3	A	999	FTC	C18-C13	2.30	1.41	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FTC	C3-N2-C1	5.35	122.85	117.83
3	A	999	FTC	C15-N14-C13	4.24	123.17	117.79
3	A	999	FTC	C16-C15-N14	-3.95	119.13	123.97
3	A	999	FTC	O17-C17-C18	3.69	121.49	115.92
3	A	999	FTC	C4-C3-N2	-3.67	117.55	122.26
3	A	999	FTC	N8-C1-N2	3.35	124.92	114.87
3	A	999	FTC	O17-C17-C16	-2.80	117.85	123.95
3	A	999	FTC	C6-C5-C4	2.69	121.95	119.24
3	A	999	FTC	CA-O17-C17	-2.49	112.99	118.08
3	A	999	FTC	C6-C1-N8	-2.42	115.85	123.02
3	A	999	FTC	C6-C1-N2	-2.33	119.07	122.61

There are no chirality outliers.

All (5) torsion outliers are listed below:

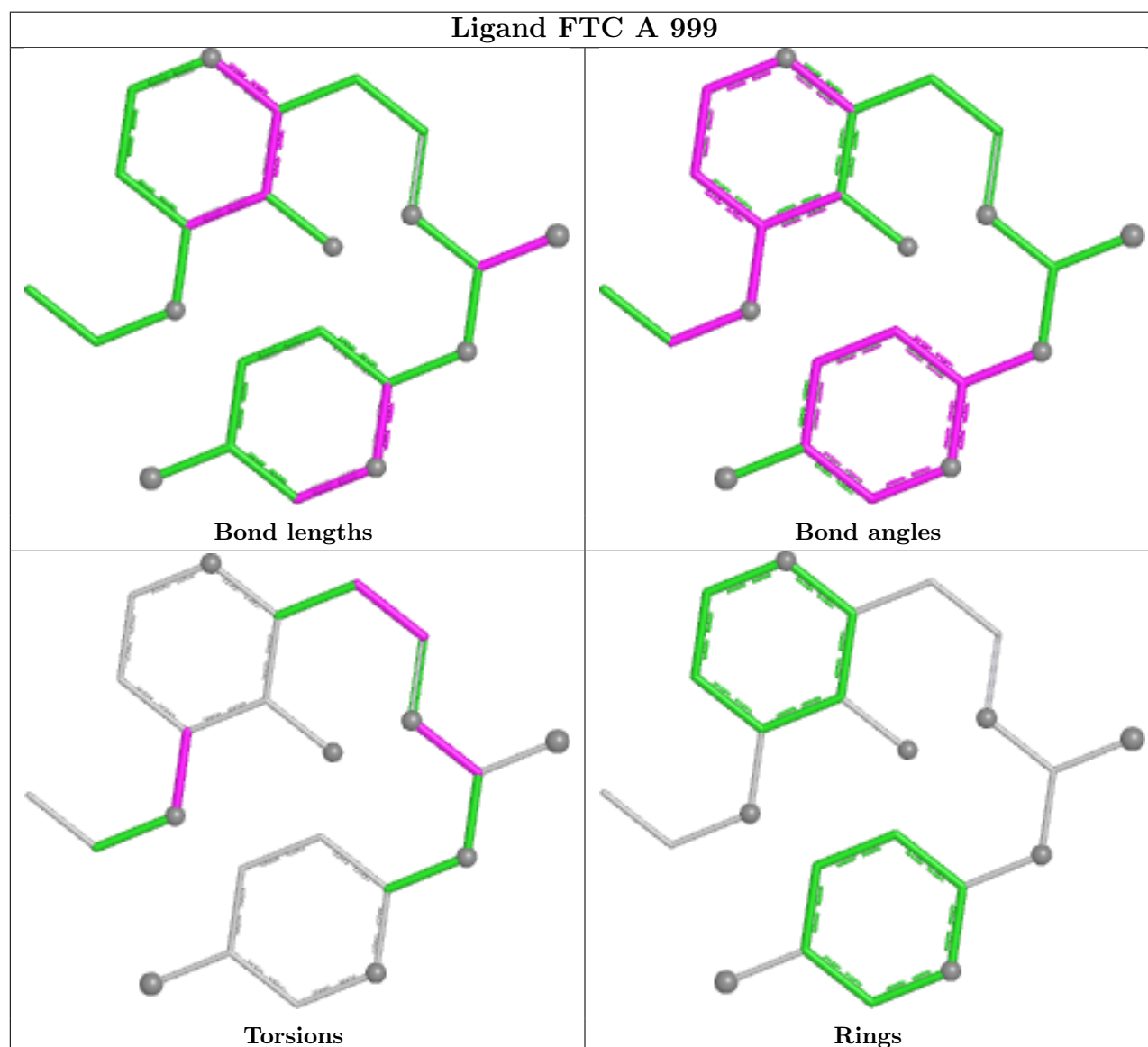
Mol	Chain	Res	Type	Atoms
3	A	999	FTC	N8-C9-N10-C11
3	A	999	FTC	C18-C17-O17-CA
3	A	999	FTC	S9-C9-N10-C11
3	A	999	FTC	N10-C11-C12-C13
3	A	999	FTC	C16-C17-O17-CA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FTC	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	280:CSD	C	281:LYS	N	2.66

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	540/560 (96%)	-0.51	0 100 100	26, 82, 148, 150	0
2	B	412/440 (93%)	-0.63	0 100 100	38, 76, 143, 150	0
All	All	952/1000 (95%)	-0.57	0 100 100	26, 80, 147, 150	0

There are no RSRZ outliers to report.

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	0.06	65,80,84,87	0

6.3 Carbohydrates [i](#)

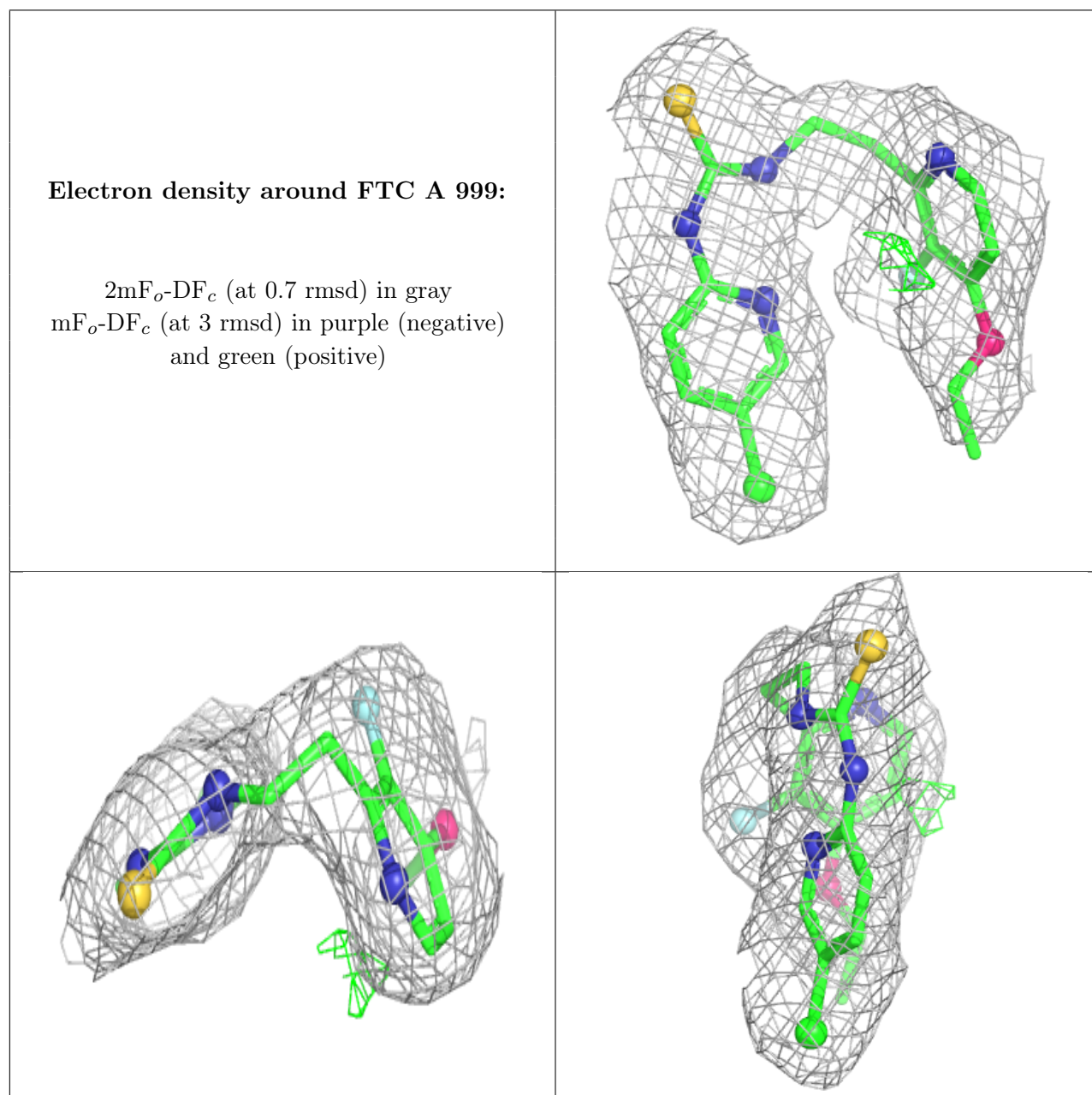
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	FTC	A	999	23/23	0.96	0.06	34,47,69,71	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 ⓘ

There are no such residues in this entry.