



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 PM UTC

PDB ID : 1JLQ / pdb_00001jlq
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH 739W94
Authors : Ren, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2001-07-16
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

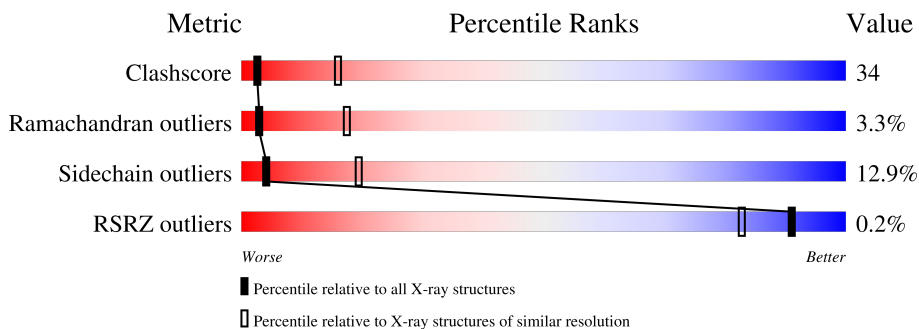
1 Overall quality at a glance

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	35% 48% 12% • 5%
2	B	440	41% 39% 11% • 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7722 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	534	Total	C	N	O	S	0	0	0
			4363	2823	724	808	8			

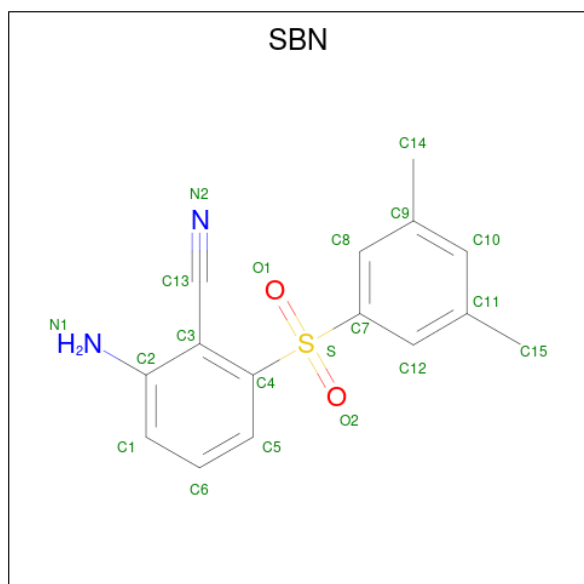
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3339	2170	556	606	7			

- Molecule 3 is 2-AMINO-6-(3,5-DIMETHYLPHENYL)SULFONYLBENZONITRILE (CCD ID: SBN) (formula: $C_{15}H_{14}N_2O_2S$).

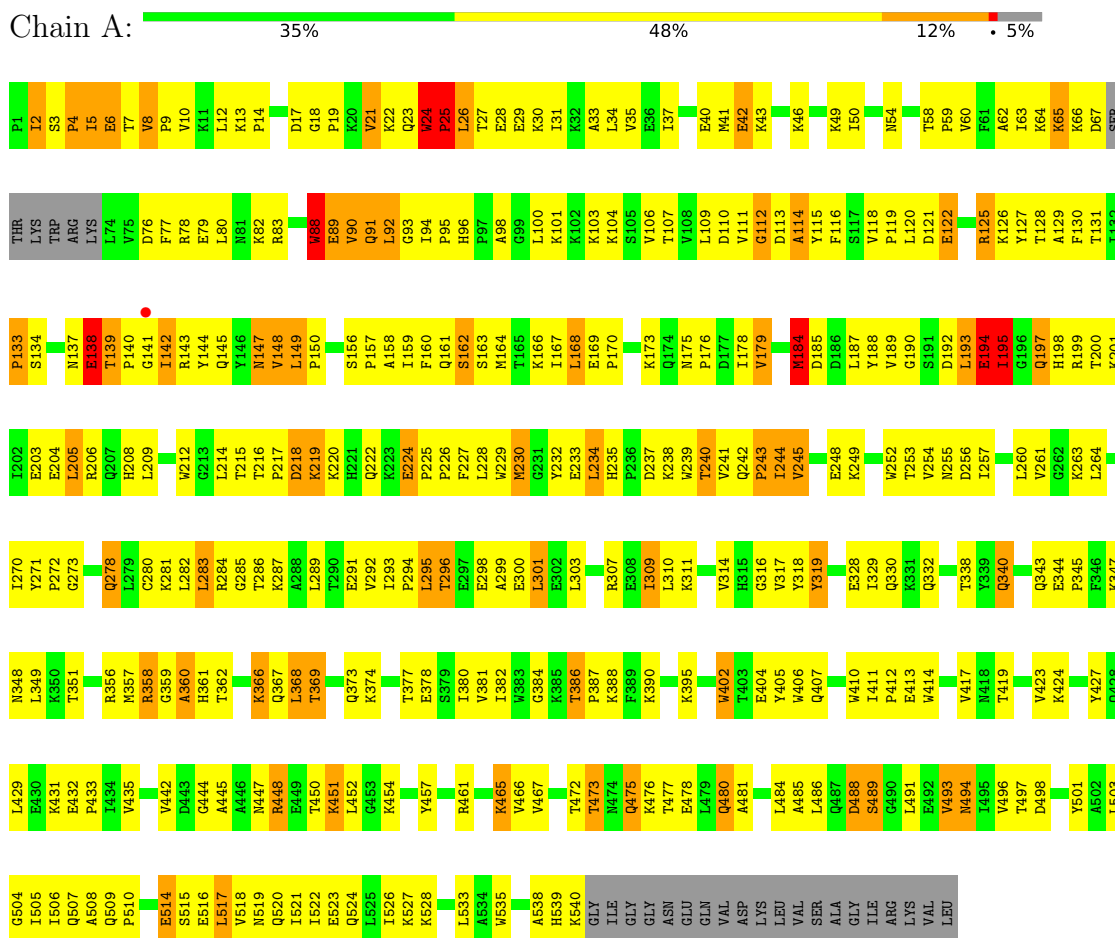


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	15	2	2	1		

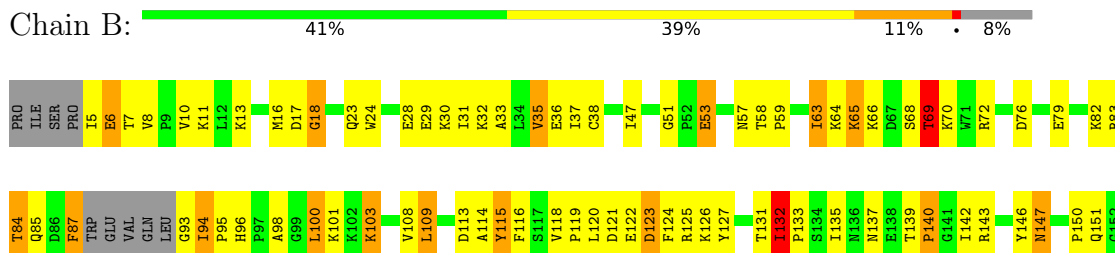
3 Residue-property plots

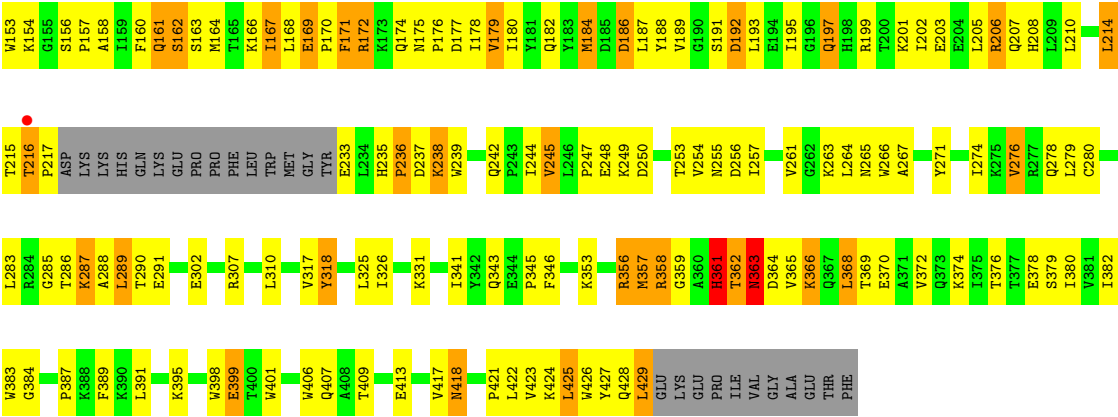
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	141.10Å 110.90Å 73.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.88-3.00) 95.7 (29.88-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.267 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.3	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	7722	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.59	0/4469	1.11	39/6074 (0.6%)
2	B	0.55	0/3431	1.09	24/4660 (0.5%)
All	All	0.57	0/7900	1.10	63/10734 (0.6%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	238	LYS	N-CA-C	-13.73	96.53	113.28
1	A	388	LYS	N-CA-C	-9.19	95.71	110.32
1	A	273	GLY	N-CA-C	-8.77	104.20	113.58
1	A	491	LEU	N-CA-C	8.70	122.88	111.75
2	B	118	VAL	N-CA-C	8.19	116.64	109.02
1	A	386	THR	CA-C-N	8.07	128.00	119.85
1	A	386	THR	C-N-CA	8.07	128.00	119.85
1	A	473	THR	N-CA-C	7.96	118.74	108.24
1	A	271	TYR	CA-C-N	-7.79	112.32	120.03
1	A	271	TYR	C-N-CA	-7.79	112.32	120.03
1	A	224	GLU	CA-C-N	7.42	128.03	120.38
1	A	224	GLU	C-N-CA	7.42	128.03	120.38
1	A	539	HIS	N-CA-C	7.33	122.17	113.23
1	A	114	ALA	N-CA-C	-7.33	104.14	113.23
1	A	489	SER	N-CA-C	7.32	122.63	112.45
2	B	250	ASP	N-CA-C	-7.31	103.32	112.90
1	A	89	GLU	N-CA-C	7.21	120.54	108.20
1	A	141	GLY	N-CA-C	-7.21	100.08	111.18
1	A	244	ILE	N-CA-C	7.11	118.84	108.53
1	A	348	ASN	N-CA-C	6.78	120.32	110.28
1	A	234	LEU	N-CA-C	6.67	119.56	108.96
1	A	402	TRP	N-CA-C	6.58	118.45	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	147	ASN	N-CA-C	-6.52	105.89	114.31
2	B	131	THR	N-CA-C	6.45	119.67	108.76
1	A	184	MET	CB-CA-C	-6.37	108.56	117.23
1	A	494	ASN	N-CA-C	-6.11	97.88	108.69
2	B	343	GLN	N-CA-C	-6.06	105.80	113.43
2	B	38	CYS	N-CA-C	6.04	119.11	111.69
2	B	171	PHE	N-CA-C	-6.00	104.86	111.82
1	A	179	VAL	N-CA-C	5.97	115.33	106.85
1	A	319	TYR	N-CA-C	5.96	118.44	108.96
2	B	391	LEU	N-CA-C	5.93	118.22	109.62
1	A	149	LEU	CA-C-N	5.90	126.36	119.99
1	A	149	LEU	C-N-CA	5.90	126.36	119.99
1	A	131	THR	N-CA-C	5.88	119.07	109.24
2	B	115	TYR	N-CA-C	5.81	118.08	111.11
2	B	192	ASP	N-CA-C	-5.73	106.29	113.28
1	A	193	LEU	N-CA-C	-5.68	102.88	110.55
2	B	271	TYR	CA-C-N	5.68	125.30	119.56
2	B	271	TYR	C-N-CA	5.68	125.30	119.56
1	A	219	LYS	N-CA-C	-5.66	105.47	112.38
2	B	428	GLN	N-CA-C	-5.62	106.13	112.87
2	B	132	ILE	CA-C-N	5.59	125.56	120.03
2	B	132	ILE	C-N-CA	5.59	125.56	120.03
1	A	343	GLN	N-CA-C	-5.57	106.54	113.55
1	A	249	LYS	N-CA-C	5.49	117.13	108.96
1	A	404	GLU	N-CA-C	5.41	120.55	113.30
2	B	417	VAL	N-CA-C	5.40	120.57	109.34
2	B	69	THR	N-CA-C	-5.39	105.44	112.23
2	B	363	ASN	N-CA-C	5.38	117.85	108.76
1	A	232	TYR	N-CA-C	5.35	118.31	109.85
2	B	366	LYS	N-CA-C	-5.30	104.55	111.02
1	A	194	GLU	N-CA-C	-5.29	102.65	110.48
2	B	18	GLY	CA-C-N	5.27	125.03	119.76
2	B	18	GLY	C-N-CA	5.27	125.03	119.76
1	A	366	LYS	N-CA-C	-5.21	105.49	111.07
1	A	245	VAL	N-CA-C	5.18	115.76	108.36
2	B	140	PRO	N-CA-C	-5.16	103.44	111.13
1	A	224	GLU	N-CA-C	5.06	117.83	109.58
2	B	153	TRP	N-CA-C	-5.04	102.30	110.32
1	A	54	ASN	CA-C-N	5.02	126.03	120.45
1	A	54	ASN	C-N-CA	5.02	126.03	120.45
1	A	147	ASN	N-CA-C	-5.00	105.88	112.94

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	4363	0	4405	334	0
2	B	3339	0	3379	205	0
3	A	20	0	14	3	0
All	All	7722	0	7798	528	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 34.

All (528) 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:358:ARG:HH11	1:A:514:GLU:HA	1.11	1.14
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.43	1.00
1:A:358:ARG:NH1	1:A:514:GLU:HA	1.77	0.99
1:A:451:LYS:HG3	1:A:472:THR:O	1.66	0.95
1:A:23:GLN:HE22	1:A:60:VAL:H	1.15	0.94
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.03	0.93
1:A:2:ILE:HG22	1:A:3:SER:H	1.35	0.91
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.52	0.90
2:B:244:ILE:HG23	2:B:429:LEU:HD23	1.53	0.90
1:A:332:GLN:NE2	1:A:332:GLN:HA	1.86	0.90
1:A:332:GLN:HA	1:A:332:GLN:HE21	1.36	0.86
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.59	0.85
2:B:5:ILE:HG22	2:B:6:GLU:H	1.41	0.84
1:A:184:MET:HE3	1:A:184:MET:HA	1.60	0.82
1:A:129:ALA:HB1	1:A:143:ARG:NH2	1.95	0.82
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.14	0.81
2:B:84:THR:HG22	2:B:154:LYS:HE2	1.63	0.81
2:B:172:ARG:HH21	2:B:176:PRO:HA	1.46	0.81
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.62	0.80
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.63	0.80
1:A:96:HIS:HD2	1:A:98:ALA:H	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:H	1:A:65:LYS:HD3	1.48	0.78
1:A:356:ARG:HB2	1:A:367:GLN:HE22	1.48	0.77
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.00	0.76
2:B:318:TYR:HD2	2:B:318:TYR:O	1.67	0.76
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.01	0.76
1:A:122:GLU:H	1:A:122:GLU:CD	1.94	0.76
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.66	0.76
2:B:374:LYS:HA	2:B:374:LYS:HE2	1.68	0.76
1:A:134:SER:HB2	1:A:137:ASN:HA	1.69	0.75
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.01	0.75
1:A:522:ILE:O	1:A:526:ILE:HG13	1.87	0.75
2:B:158:ALA:O	2:B:161:GLN:HB2	1.87	0.75
2:B:170:PRO:O	2:B:174:GLN:HG2	1.85	0.74
2:B:203:GLU:HA	2:B:206:ARG:HD2	1.69	0.74
2:B:244:ILE:CG2	2:B:429:LEU:HD23	2.17	0.74
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.69	0.74
2:B:197:GLN:O	2:B:201:LYS:HB2	1.87	0.73
2:B:157:PRO:HG2	2:B:184:MET:HA	1.71	0.73
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.71	0.73
1:A:65:LYS:HD3	1:A:65:LYS:N	2.05	0.71
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.55	0.71
1:A:27:THR:HG22	1:A:28:GLU:N	2.05	0.71
2:B:206:ARG:O	2:B:210:LEU:HD13	1.90	0.71
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.89	0.71
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.26	0.71
1:A:27:THR:HG22	1:A:29:GLU:H	1.56	0.70
2:B:235:HIS:O	2:B:238:LYS:HB2	1.91	0.70
2:B:421:PRO:O	2:B:425:LEU:HD22	1.91	0.70
1:A:282:LEU:HD12	1:A:293:ILE:CG2	2.22	0.70
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.27	0.69
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.21	0.69
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.74	0.69
1:A:23:GLN:O	1:A:25:PRO:HD3	1.92	0.69
1:A:96:HIS:CD2	1:A:98:ALA:H	2.10	0.69
1:A:472:THR:O	1:A:473:THR:HG23	1.93	0.69
1:A:378:GLU:O	1:A:382:ILE:HG13	1.93	0.69
1:A:507:GLN:C	1:A:509:GLN:H	2.00	0.68
2:B:79:GLU:O	2:B:83:ARG:HG3	1.94	0.68
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.75	0.67
1:A:252:TRP:CD1	1:A:295:LEU:HD12	2.29	0.67
2:B:203:GLU:HA	2:B:206:ARG:CD	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HB	1:A:140:PRO:CD	2.25	0.67
1:A:451:LYS:CG	1:A:472:THR:O	2.42	0.67
1:A:199:ARG:HG3	1:A:219:LYS:HZ3	1.58	0.67
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.77	0.67
1:A:454:LYS:HA	1:A:467:VAL:O	1.95	0.67
1:A:503:LEU:HD23	1:A:535:TRP:HB2	1.77	0.67
2:B:395:LYS:O	2:B:399:GLU:HG2	1.94	0.67
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.30	0.67
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.76	0.66
1:A:205:LEU:O	1:A:208:HIS:HB3	1.95	0.66
1:A:235:HIS:HB2	1:A:238:LYS:O	1.94	0.66
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.09	0.66
2:B:93:GLY:O	2:B:94:ILE:HG22	1.96	0.66
1:A:139:THR:HB	1:A:140:PRO:HD3	1.78	0.66
1:A:282:LEU:HD12	1:A:293:ILE:HG21	1.77	0.65
1:A:134:SER:HB3	1:A:138:GLU:OE2	1.96	0.65
2:B:66:LYS:C	2:B:68:SER:H	2.04	0.65
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.78	0.65
2:B:365:VAL:O	2:B:369:THR:HG23	1.96	0.65
1:A:257:ILE:O	1:A:261:VAL:HG23	1.96	0.65
1:A:5:ILE:HD12	1:A:6:GLU:OE1	1.96	0.65
1:A:12:LEU:HD22	1:A:83:ARG:HB3	1.79	0.65
1:A:457:TYR:HE2	1:A:465:LYS:HD2	1.61	0.65
2:B:5:ILE:HG22	2:B:6:GLU:N	2.12	0.65
1:A:244:ILE:CG2	1:A:310:LEU:HD13	2.27	0.64
2:B:63:ILE:HD13	2:B:63:ILE:H	1.62	0.64
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.32	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.64
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.33	0.64
1:A:24:TRP:O	1:A:25:PRO:C	2.40	0.64
1:A:89:GLU:OE1	1:A:92:LEU:HD22	1.98	0.64
1:A:503:LEU:HD13	1:A:533:LEU:HG	1.79	0.64
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.80	0.64
1:A:104:LYS:HD2	1:A:192:ASP:O	1.97	0.64
1:A:366:LYS:O	1:A:369:THR:HB	1.98	0.64
1:A:507:GLN:O	1:A:509:GLN:N	2.30	0.64
2:B:179:VAL:O	2:B:180:ILE:HD12	1.97	0.64
2:B:380:ILE:O	2:B:384:GLY:N	2.30	0.64
1:A:2:ILE:HG22	1:A:3:SER:N	2.11	0.63
1:A:58:THR:HG23	1:A:76:ASP:O	1.99	0.63
1:A:199:ARG:HD3	1:A:219:LYS:HZ1	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:N	1:A:142:ILE:HD12	2.14	0.62
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.33	0.62
1:A:260:LEU:O	1:A:264:LEU:HD23	1.99	0.62
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.82	0.61
1:A:244:ILE:CG2	1:A:310:LEU:HD22	2.30	0.61
1:A:384:GLY:HA3	2:B:135:ILE:HD13	1.83	0.61
1:A:292:VAL:C	1:A:293:ILE:HD12	2.25	0.61
1:A:33:ALA:O	1:A:37:ILE:HD13	1.99	0.61
2:B:172:ARG:NH2	2:B:178:ILE:O	2.29	0.61
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.83	0.60
1:A:317:VAL:HG12	1:A:318:TYR:O	2.01	0.60
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.16	0.60
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.82	0.60
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.66	0.60
1:A:300:GLU:OE2	1:A:300:GLU:HA	2.00	0.60
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.81	0.60
2:B:356:ARG:HH12	2:B:359:GLY:H	1.48	0.60
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.81	0.60
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.83	0.60
1:A:94:ILE:HG23	1:A:229:TRP:HZ2	1.66	0.60
1:A:91:GLN:HE21	1:A:94:ILE:HD11	1.67	0.60
2:B:206:ARG:C	2:B:210:LEU:HD13	2.26	0.60
2:B:100:LEU:HD23	2:B:100:LEU:H	1.66	0.60
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.84	0.60
2:B:182:GLN:HA	2:B:187:LEU:HD12	1.82	0.59
2:B:368:LEU:O	2:B:372:VAL:HG23	2.02	0.59
2:B:214:LEU:N	2:B:214:LEU:HD23	2.16	0.59
2:B:245:VAL:O	2:B:429:LEU:HG	2.02	0.59
2:B:345:PRO:O	2:B:346:PHE:HB2	2.02	0.59
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.84	0.59
1:A:507:GLN:C	1:A:509:GLN:N	2.58	0.59
1:A:37:ILE:O	1:A:40:GLU:HB3	2.02	0.59
1:A:116:PHE:O	1:A:148:VAL:HG21	2.02	0.59
1:A:168:LEU:HD11	1:A:209:LEU:HD21	1.85	0.59
1:A:501:TYR:CE2	1:A:505:ILE:HD11	2.36	0.59
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.38	0.59
1:A:106:VAL:HG11	3:A:999:SBN:C5	2.32	0.59
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.02	0.59
2:B:424:LYS:HD2	2:B:424:LYS:O	2.02	0.59
2:B:123:ASP:O	2:B:126:LYS:HE3	2.03	0.59
1:A:219:LYS:HA	1:A:222:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.85	0.59
2:B:182:GLN:HB2	2:B:187:LEU:HD11	1.84	0.58
2:B:395:LYS:O	2:B:399:GLU:CG	2.50	0.58
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	0.58
1:A:517:LEU:O	1:A:520:GLN:HB2	2.03	0.58
1:A:229:TRP:O	1:A:230:MET:C	2.47	0.58
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.33	0.58
1:A:46:LYS:HE3	1:A:116:PHE:CD2	2.39	0.57
1:A:356:ARG:CB	1:A:367:GLN:NE2	2.67	0.57
1:A:402:TRP:HZ3	2:B:364:ASP:OD2	1.87	0.57
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.39	0.57
1:A:66:LYS:HG3	1:A:67:ASP:H	1.68	0.57
1:A:478:GLU:O	1:A:481:ALA:HB3	2.03	0.57
2:B:236:PRO:C	2:B:238:LYS:H	2.13	0.57
1:A:27:THR:CG2	1:A:28:GLU:N	2.68	0.57
1:A:270:ILE:O	1:A:272:PRO:HD3	2.04	0.57
1:A:503:LEU:O	1:A:504:GLY:C	2.46	0.57
2:B:236:PRO:O	2:B:238:LYS:N	2.37	0.57
1:A:22:LYS:HG2	1:A:23:GLN:N	2.18	0.57
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.69	0.57
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.86	0.57
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.70	0.56
2:B:163:SER:O	2:B:167:ILE:HG13	2.05	0.56
2:B:175:ASN:N	2:B:176:PRO:HD3	2.20	0.56
2:B:288:ALA:O	2:B:291:GLU:HB3	2.04	0.56
1:A:252:TRP:CD1	1:A:295:LEU:CD1	2.88	0.56
1:A:17:ASP:O	1:A:83:ARG:HD3	2.06	0.56
2:B:254:VAL:HG21	2:B:288:ALA:O	2.05	0.56
2:B:261:VAL:HG13	2:B:276:VAL:CG2	2.35	0.56
1:A:27:THR:HG22	1:A:28:GLU:H	1.69	0.55
1:A:253:THR:O	1:A:256:ASP:HB2	2.06	0.55
2:B:254:VAL:HB	2:B:289:LEU:HA	1.89	0.55
2:B:16:MET:HE3	2:B:83:ARG:HA	1.89	0.55
2:B:167:ILE:O	2:B:208:HIS:NE2	2.40	0.55
1:A:111:VAL:HG11	1:A:187:LEU:HD22	1.89	0.55
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.89	0.55
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.89	0.55
1:A:122:GLU:HA	1:A:125:ARG:NE	2.22	0.55
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.37	0.55
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.07	0.54
2:B:100:LEU:H	2:B:100:LEU:CD2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HG21	1:A:310:LEU:HD22	1.89	0.54
2:B:406:TRP:O	2:B:407:GLN:HG3	2.07	0.54
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.73	0.54
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.38	0.54
2:B:318:TYR:O	2:B:318:TYR:CD2	2.55	0.54
2:B:341:ILE:N	2:B:341:ILE:HD12	2.22	0.54
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.43	0.54
1:A:27:THR:HB	1:A:30:LYS:HG3	1.89	0.54
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.36	0.54
1:A:120:LEU:HD12	1:A:121:ASP:N	2.22	0.54
1:A:445:ALA:N	1:A:477:THR:HG21	2.23	0.54
2:B:29:GLU:HG2	2:B:30:LYS:N	2.23	0.54
2:B:160:PHE:O	2:B:160:PHE:CD1	2.60	0.54
1:A:486:LEU:O	1:A:528:LYS:NZ	2.41	0.54
1:A:120:LEU:HD12	1:A:121:ASP:H	1.73	0.54
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.90	0.54
1:A:158:ALA:O	1:A:161:GLN:HB3	2.09	0.53
2:B:113:ASP:O	2:B:114:ALA:C	2.51	0.53
1:A:7:THR:HG22	1:A:119:PRO:HG2	1.91	0.53
1:A:516:GLU:OE2	1:A:516:GLU:HA	2.08	0.53
1:A:23:GLN:NE2	1:A:60:VAL:H	1.96	0.53
1:A:40:GLU:O	1:A:43:LYS:HG2	2.08	0.53
1:A:64:LYS:HE2	1:A:66:LYS:NZ	2.24	0.53
2:B:244:ILE:HG23	2:B:429:LEU:CD2	2.34	0.53
1:A:281:LYS:HE3	1:A:284:ARG:NH1	2.24	0.53
2:B:180:ILE:HD11	2:B:189:VAL:HG13	1.91	0.53
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.89	0.53
2:B:206:ARG:NH2	2:B:217:PRO:HA	2.23	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.96	0.53
2:B:374:LYS:O	2:B:378:GLU:HG3	2.08	0.53
1:A:110:ASP:C	1:A:112:GLY:H	2.16	0.53
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.44	0.53
1:A:503:LEU:O	1:A:507:GLN:HG2	2.09	0.53
1:A:13:LYS:HD2	1:A:82:LYS:O	2.09	0.52
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.39	0.52
2:B:66:LYS:C	2:B:68:SER:N	2.66	0.52
2:B:98:ALA:HB1	2:B:101:LYS:HD3	1.91	0.52
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.44	0.52
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.39	0.52
2:B:423:VAL:O	2:B:427:TYR:HD2	1.92	0.52
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:CG2	1:A:28:GLU:H	2.21	0.52
1:A:41:MET:HB3	1:A:46:LYS:NZ	2.25	0.52
2:B:101:LYS:NZ	2:B:101:LYS:HB3	2.24	0.52
2:B:383:TRP:O	2:B:384:GLY:C	2.53	0.52
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.75	0.52
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.91	0.52
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.92	0.52
2:B:120:LEU:HD21	2:B:124:PHE:HD2	1.75	0.52
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.45	0.52
1:A:518:VAL:O	1:A:522:ILE:HG13	2.10	0.51
2:B:100:LEU:HD23	2:B:100:LEU:N	2.25	0.51
2:B:120:LEU:HD23	2:B:121:ASP:O	2.11	0.51
2:B:326:ILE:O	2:B:341:ILE:HA	2.10	0.51
2:B:413:GLU:HA	2:B:413:GLU:OE2	2.10	0.51
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.46	0.51
1:A:134:SER:HB2	1:A:137:ASN:CA	2.39	0.51
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.26	0.51
2:B:361:HIS:HD2	2:B:362:THR:HG22	1.76	0.51
1:A:184:MET:HA	1:A:184:MET:CE	2.37	0.51
2:B:58:THR:HG23	2:B:76:ASP:O	2.10	0.51
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.40	0.51
1:A:498:ASP:C	1:A:535:TRP:HE1	2.18	0.51
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.91	0.51
1:A:445:ALA:H	1:A:477:THR:HG21	1.76	0.51
1:A:23:GLN:HE22	1:A:60:VAL:N	1.97	0.50
1:A:199:ARG:HG3	1:A:219:LYS:NZ	2.25	0.50
1:A:237:ASP:OD2	1:A:237:ASP:N	2.43	0.50
1:A:254:VAL:O	1:A:255:ASN:C	2.53	0.50
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.77	0.50
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.27	0.50
2:B:126:LYS:HG3	2:B:127:TYR:N	2.26	0.50
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.12	0.50
1:A:94:ILE:HG23	1:A:229:TRP:CZ2	2.45	0.50
1:A:96:HIS:HD2	1:A:98:ALA:N	2.03	0.50
1:A:283:LEU:O	1:A:286:THR:HG23	2.12	0.50
1:A:106:VAL:HG11	3:A:999:SBN:H5	1.94	0.50
1:A:188:TYR:CD1	1:A:188:TYR:N	2.80	0.50
1:A:427:TYR:CE2	1:A:509:GLN:HG2	2.47	0.50
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.94	0.50
1:A:285:GLY:O	1:A:286:THR:C	2.55	0.50
1:A:318:TYR:O	1:A:349:LEU:HD21	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:CZ3	2:B:364:ASP:OD2	2.65	0.49
2:B:206:ARG:CZ	2:B:216:THR:O	2.59	0.49
2:B:317:VAL:HG23	2:B:317:VAL:O	2.12	0.49
1:A:301:LEU:HD12	1:A:301:LEU:O	2.12	0.49
2:B:286:THR:O	2:B:286:THR:OG1	2.26	0.49
1:A:358:ARG:NH1	1:A:514:GLU:CA	2.65	0.49
2:B:64:LYS:NZ	2:B:69:THR:O	2.37	0.49
1:A:64:LYS:CE	1:A:66:LYS:HZ3	2.25	0.49
1:A:88:TRP:CG	1:A:89:GLU:H	2.29	0.49
1:A:233:GLU:CB	1:A:240:THR:HG22	2.43	0.49
1:A:50:ILE:HG23	1:A:145:GLN:HG2	1.95	0.49
1:A:90:VAL:O	1:A:91:GLN:HB2	2.12	0.49
1:A:332:GLN:HE21	1:A:332:GLN:CA	2.08	0.49
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.41	0.49
1:A:296:THR:HG23	1:A:299:ALA:CB	2.41	0.49
1:A:241:VAL:O	1:A:243:PRO:N	2.46	0.49
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.94	0.49
1:A:90:VAL:O	1:A:91:GLN:CB	2.60	0.49
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.47	0.49
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.48	0.49
2:B:422:LEU:C	2:B:424:LYS:N	2.69	0.49
1:A:377:THR:O	1:A:381:VAL:HG23	2.13	0.49
2:B:125:ARG:NE	2:B:147:ASN:HA	2.26	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	3.01	0.49
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.30	0.49
1:A:179:VAL:O	1:A:189:VAL:HA	2.13	0.48
1:A:239:TRP:HZ3	1:A:241:VAL:HG23	1.78	0.48
2:B:424:LYS:HD2	2:B:424:LYS:C	2.38	0.48
1:A:94:ILE:HG22	1:A:95:PRO:O	2.13	0.48
2:B:157:PRO:CG	2:B:184:MET:HA	2.40	0.48
2:B:363:ASN:OD1	2:B:363:ASN:C	2.56	0.48
1:A:332:GLN:HG2	1:A:338:THR:HG23	1.95	0.48
2:B:236:PRO:C	2:B:238:LYS:N	2.71	0.48
1:A:134:SER:HB3	1:A:138:GLU:HG2	1.95	0.48
1:A:194:GLU:O	1:A:195:ILE:C	2.56	0.48
1:A:203:GLU:O	1:A:204:GLU:C	2.56	0.48
1:A:46:LYS:HE3	1:A:116:PHE:HD2	1.79	0.48
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.48	0.48
1:A:410:TRP:HZ3	2:B:401:TRP:CE2	2.31	0.48
2:B:33:ALA:O	2:B:37:ILE:HG13	2.14	0.48
2:B:427:TYR:C	2:B:429:LEU:N	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:OG1	1:A:473:THR:N	2.40	0.48
2:B:193:LEU:H	2:B:193:LEU:CD1	2.27	0.48
1:A:195:ILE:O	1:A:198:HIS:HB3	2.13	0.48
1:A:218:ASP:C	1:A:220:LYS:N	2.70	0.48
2:B:427:TYR:C	2:B:429:LEU:H	2.22	0.47
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.29	0.47
1:A:58:THR:CG2	1:A:76:ASP:O	2.62	0.47
1:A:270:ILE:C	1:A:272:PRO:HD3	2.40	0.47
1:A:37:ILE:HD12	1:A:37:ILE:H	1.78	0.47
2:B:63:ILE:HD13	2:B:63:ILE:N	2.27	0.47
1:A:107:THR:HG21	1:A:222:GLN:OE1	2.14	0.47
1:A:367:GLN:O	1:A:368:LEU:C	2.58	0.47
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.97	0.47
2:B:376:THR:HG23	2:B:387:PRO:HD2	1.96	0.47
1:A:118:VAL:HB	1:A:149:LEU:HG	1.97	0.47
1:A:122:GLU:HA	1:A:125:ARG:HE	1.79	0.47
1:A:142:ILE:N	1:A:142:ILE:CD1	2.78	0.47
2:B:53:GLU:CD	2:B:53:GLU:H	2.22	0.47
1:A:65:LYS:HG2	1:A:65:LYS:O	2.14	0.47
1:A:93:GLY:O	2:B:137:ASN:CB	2.62	0.47
1:A:515:SER:CB	1:A:518:VAL:HG23	2.44	0.47
2:B:79:GLU:HA	2:B:82:LYS:HE2	1.97	0.47
2:B:356:ARG:CZ	2:B:361:HIS:HB3	2.45	0.47
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.15	0.47
1:A:199:ARG:CD	1:A:219:LYS:HZ1	2.26	0.47
1:A:293:ILE:HD12	1:A:293:ILE:N	2.30	0.47
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.50	0.47
2:B:175:ASN:C	2:B:177:ASP:H	2.23	0.47
2:B:206:ARG:HH11	2:B:206:ARG:HB3	1.80	0.47
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.50	0.47
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.15	0.47
1:A:137:ASN:O	1:A:138:GLU:O	2.33	0.47
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.97	0.47
2:B:205:LEU:HD13	2:B:205:LEU:C	2.40	0.47
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.51	0.46
1:A:163:SER:O	1:A:167:ILE:HG13	2.15	0.46
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.96	0.46
1:A:244:ILE:HG21	1:A:310:LEU:HD13	1.96	0.46
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.31	0.46
1:A:42:GLU:OE2	1:A:49:LYS:HE3	2.15	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:GLN:HA	2:B:210:LEU:HD22	1.98	0.46
2:B:285:GLY:O	2:B:287:LYS:HG2	2.16	0.46
1:A:115:TYR:O	1:A:149:LEU:HB2	2.15	0.46
1:A:419:THR:HG23	1:A:419:THR:O	2.16	0.46
1:A:83:ARG:NH1	1:A:83:ARG:HG3	2.31	0.45
1:A:488:ASP:OD2	1:A:488:ASP:N	2.50	0.45
2:B:422:LEU:C	2:B:424:LYS:H	2.23	0.45
1:A:3:SER:HB2	1:A:212:TRP:O	2.17	0.45
1:A:427:TYR:O	1:A:509:GLN:NE2	2.48	0.45
2:B:357:MET:HB2	2:B:370:GLU:OE1	2.16	0.45
1:A:110:ASP:C	1:A:112:GLY:N	2.73	0.45
1:A:493:VAL:HG12	1:A:494:ASN:H	1.81	0.45
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.45
1:A:317:VAL:HG12	1:A:318:TYR:N	2.30	0.45
1:A:417:VAL:HG13	1:A:417:VAL:O	2.16	0.45
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.47	0.45
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.32	0.45
2:B:11:LYS:HE3	2:B:85:GLN:HE21	1.81	0.45
2:B:98:ALA:HA	2:B:101:LYS:CD	2.47	0.45
1:A:118:VAL:O	1:A:148:VAL:HG22	2.17	0.45
2:B:98:ALA:HA	2:B:101:LYS:HD2	1.99	0.45
2:B:179:VAL:C	2:B:180:ILE:HD12	2.41	0.45
1:A:199:ARG:CD	1:A:219:LYS:NZ	2.80	0.45
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.80	0.45
1:A:480:GLN:NE2	1:A:484:LEU:HG	2.32	0.45
1:A:317:VAL:CG1	1:A:318:TYR:N	2.79	0.45
1:A:359:GLY:O	1:A:360:ALA:C	2.59	0.45
2:B:253:THR:O	2:B:257:ILE:HG12	2.16	0.45
1:A:139:THR:CB	1:A:140:PRO:CD	2.95	0.45
1:A:309:ILE:HG22	1:A:310:LEU:N	2.32	0.45
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.99	0.45
1:A:489:SER:OG	1:A:528:LYS:NZ	2.46	0.45
2:B:35:VAL:HG12	2:B:36:GLU:N	2.30	0.45
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.45
2:B:162:SER:O	2:B:163:SER:C	2.59	0.45
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.98	0.44
1:A:344:GLU:HB2	1:A:347:LYS:HD3	1.98	0.44
1:A:373:GLN:HG3	1:A:374:LYS:N	2.32	0.44
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.52	0.44
2:B:116:PHE:CE2	2:B:151:GLN:NE2	2.82	0.44
1:A:26:LEU:HB3	1:A:30:LYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:O	1:A:128:THR:OG1	2.31	0.44
1:A:65:LYS:H	1:A:65:LYS:CD	2.25	0.44
1:A:472:THR:O	1:A:473:THR:CG2	2.63	0.44
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.61	0.44
1:A:5:ILE:HD11	1:A:166:LYS:NZ	2.31	0.44
1:A:88:TRP:CG	1:A:89:GLU:N	2.83	0.44
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.00	0.44
1:A:344:GLU:O	1:A:345:PRO:C	2.59	0.44
1:A:356:ARG:HE	1:A:374:LYS:NZ	2.16	0.44
1:A:503:LEU:CD1	1:A:533:LEU:HG	2.44	0.44
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.00	0.44
1:A:103:LYS:HE3	1:A:179:VAL:HG21	2.00	0.44
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.48	0.44
2:B:94:ILE:O	2:B:94:ILE:CG2	2.65	0.44
2:B:264:LEU:O	2:B:265:ASN:C	2.60	0.44
1:A:466:VAL:HG22	1:A:467:VAL:N	2.31	0.44
2:B:94:ILE:O	2:B:94:ILE:HG23	2.18	0.44
2:B:353:LYS:HE3	2:B:353:LYS:HB2	1.80	0.44
2:B:423:VAL:O	2:B:427:TYR:CD2	2.71	0.44
1:A:12:LEU:HD22	1:A:83:ARG:CB	2.47	0.44
1:A:23:GLN:CG	1:A:133:PRO:HD3	2.47	0.44
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.48	0.44
1:A:201:LYS:O	1:A:204:GLU:HB3	2.18	0.44
2:B:31:ILE:HD12	2:B:133:PRO:O	2.18	0.44
2:B:197:GLN:N	2:B:197:GLN:OE1	2.51	0.44
2:B:287:LYS:HG2	2:B:287:LYS:H	1.60	0.44
1:A:98:ALA:HB2	1:A:349:LEU:O	2.17	0.43
1:A:444:GLY:HA3	1:A:477:THR:HG22	2.00	0.43
1:A:8:VAL:O	1:A:10:VAL:HG23	2.17	0.43
1:A:173:LYS:O	1:A:176:PRO:HD3	2.18	0.43
1:A:332:GLN:NE2	1:A:332:GLN:CA	2.60	0.43
2:B:32:LYS:O	2:B:33:ALA:C	2.60	0.43
2:B:63:ILE:HD13	2:B:72:ARG:O	2.18	0.43
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.98	0.43
2:B:103:LYS:HE3	2:B:192:ASP:OD1	2.18	0.43
1:A:103:LYS:HE2	3:A:999:SBN:N2	2.33	0.43
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.47	0.43
1:A:317:VAL:HG21	1:A:347:LYS:HB3	2.01	0.43
1:A:106:VAL:HG12	1:A:227:PHE:HE2	1.83	0.43
2:B:202:ILE:HG22	2:B:203:GLU:N	2.34	0.43
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:VAL:HG23	2:B:132:ILE:HG21	2.01	0.43
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.18	0.43
2:B:29:GLU:CG	2:B:30:LYS:N	2.81	0.43
2:B:247:PRO:HB2	2:B:249:LYS:NZ	2.34	0.43
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.76	0.43
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.19	0.43
1:A:34:LEU:HD11	1:A:62:ALA:HB2	2.00	0.43
1:A:241:VAL:HG21	1:A:314:VAL:HB	2.01	0.43
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.33	0.43
1:A:493:VAL:HG12	1:A:494:ASN:N	2.34	0.43
2:B:189:VAL:HB	2:B:202:ILE:HD11	2.01	0.43
1:A:193:LEU:HB3	1:A:197:GLN:HB3	2.01	0.42
2:B:161:GLN:O	2:B:164:MET:HB3	2.19	0.42
1:A:64:LYS:HE2	1:A:66:LYS:HZ3	1.84	0.42
1:A:405:TYR:O	2:B:331:LYS:HD3	2.19	0.42
1:A:412:PRO:O	1:A:413:GLU:C	2.61	0.42
1:A:480:GLN:O	1:A:481:ALA:C	2.62	0.42
1:A:497:THR:O	1:A:535:TRP:HA	2.18	0.42
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.19	0.42
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.53	0.42
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.19	0.42
1:A:106:VAL:HG12	1:A:107:THR:N	2.34	0.42
2:B:116:PHE:CZ	2:B:151:GLN:NE2	2.87	0.42
1:A:233:GLU:HB2	1:A:240:THR:HG22	2.01	0.42
2:B:17:ASP:OD1	2:B:18:GLY:N	2.50	0.42
2:B:96:HIS:NE2	2:B:382:ILE:O	2.46	0.42
1:A:233:GLU:HB3	1:A:240:THR:HG22	2.02	0.42
2:B:358:ARG:H	2:B:358:ARG:CD	2.33	0.42
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.50	0.42
1:A:103:LYS:HD2	1:A:190:GLY:HA3	2.01	0.42
1:A:226:PRO:HA	1:A:234:LEU:O	2.19	0.42
2:B:87:PHE:CD1	2:B:87:PHE:N	2.88	0.42
2:B:132:ILE:HB	2:B:142:ILE:HB	2.02	0.42
2:B:195:ILE:HG12	2:B:199:ARG:CZ	2.49	0.42
2:B:239:TRP:CZ3	2:B:378:GLU:HB3	2.55	0.42
2:B:255:ASN:O	2:B:256:ASP:C	2.61	0.42
1:A:169:GLU:N	1:A:170:PRO:HD2	2.35	0.42
2:B:202:ILE:O	2:B:205:LEU:N	2.53	0.42
1:A:465:LYS:HG2	1:A:466:VAL:N	2.35	0.42
2:B:254:VAL:CG2	2:B:288:ALA:O	2.68	0.42
1:A:498:ASP:C	1:A:535:TRP:NE1	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:HE2	2:B:72:ARG:HD3	2.02	0.41
2:B:168:LEU:O	2:B:169:GLU:C	2.63	0.41
1:A:254:VAL:HG13	1:A:283:LEU:HD12	2.03	0.41
1:A:465:LYS:CG	1:A:466:VAL:N	2.83	0.41
2:B:109:LEU:O	2:B:186:ASP:HA	2.19	0.41
1:A:162:SER:O	1:A:163:SER:C	2.63	0.41
2:B:325:LEU:HD12	2:B:325:LEU:HA	1.93	0.41
1:A:114:ALA:HB3	1:A:160:PHE:HE2	1.85	0.41
1:A:118:VAL:O	1:A:148:VAL:CG2	2.68	0.41
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.89	0.41
1:A:480:GLN:HE22	1:A:484:LEU:HG	1.86	0.41
2:B:193:LEU:H	2:B:193:LEU:HD12	1.85	0.41
2:B:193:LEU:HD12	2:B:193:LEU:N	2.35	0.41
1:A:64:LYS:CE	1:A:66:LYS:NZ	2.82	0.41
1:A:100:LEU:O	1:A:318:TYR:HB3	2.20	0.41
1:A:114:ALA:HB3	1:A:160:PHE:CE2	2.56	0.41
1:A:329:ILE:HG22	1:A:330:GLN:N	2.35	0.41
1:A:380:ILE:HG13	1:A:386:THR:HG22	2.02	0.41
2:B:139:THR:HG22	2:B:140:PRO:CD	2.51	0.41
1:A:91:GLN:O	1:A:92:LEU:C	2.63	0.41
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.45	0.41
1:A:120:LEU:O	1:A:121:ASP:C	2.64	0.41
2:B:51:GLY:CA	2:B:53:GLU:OE2	2.69	0.41
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.77	0.41
2:B:28:GLU:O	2:B:29:GLU:C	2.64	0.41
1:A:111:VAL:CG1	1:A:187:LEU:HB2	2.51	0.41
1:A:242:GLN:O	1:A:243:PRO:O	2.39	0.41
1:A:357:MET:O	1:A:358:ARG:C	2.63	0.41
1:A:475:GLN:O	1:A:476:LYS:C	2.63	0.41
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.51	0.41
2:B:7:THR:HG22	2:B:119:PRO:CG	2.37	0.41
2:B:422:LEU:O	2:B:424:LYS:N	2.53	0.41
1:A:427:TYR:OH	1:A:509:GLN:HA	2.20	0.41
1:A:13:LYS:HB3	1:A:14:PRO:HD2	2.03	0.40
1:A:254:VAL:HG23	1:A:291:GLU:O	2.21	0.40
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.48	0.40
2:B:5:ILE:CG2	2:B:6:GLU:H	2.21	0.40
2:B:126:LYS:CG	2:B:127:TYR:N	2.84	0.40
2:B:380:ILE:O	2:B:384:GLY:CA	2.69	0.40
1:A:227:PHE:O	1:A:234:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:O	1:A:242:GLN:C	2.64	0.40
1:A:411:ILE:HG22	1:A:414:TRP:CD1	2.56	0.40
1:A:503:LEU:HD12	1:A:503:LEU:HA	1.75	0.40
2:B:161:GLN:NE2	2:B:161:GLN:HA	2.36	0.40
2:B:266:TRP:CD1	2:B:422:LEU:HD13	2.56	0.40
1:A:205:LEU:O	1:A:206:ARG:C	2.64	0.40
1:A:242:GLN:O	1:A:243:PRO:C	2.64	0.40
1:A:244:ILE:HG12	1:A:245:VAL:N	2.37	0.40
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.56	0.40
1:A:509:GLN:N	1:A:510:PRO:CD	2.85	0.40
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.85	0.40
2:B:276:VAL:O	2:B:276:VAL:HG13	2.21	0.40
1:A:101:LYS:HG2	1:A:319:TYR:O	2.22	0.40
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.03	0.40
2:B:101:LYS:HB3	2:B:101:LYS:HZ3	1.86	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	529/560 (94%)	452 (85%)	58 (11%)	19 (4%)	2	16
2	B	399/440 (91%)	342 (86%)	45 (11%)	12 (3%)	3	19
All	All	928/1000 (93%)	794 (86%)	103 (11%)	31 (3%)	3	17

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	91	GLN
1	A	138	GLU

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Mol	Chain	Res	Type
1	A	195	ILE
2	B	215	THR
2	B	237	ASP
1	A	88	TRP
1	A	112	GLY
1	A	139	THR
1	A	230	MET
1	A	243	PRO
1	A	358	ARG
1	A	508	ALA
2	B	162	SER
2	B	361	HIS
1	A	24	TRP
1	A	25	PRO
1	A	125	ARG
1	A	360	ALA
2	B	236	PRO
2	B	356	ARG
2	B	94	ILE
1	A	90	VAL
2	B	103	LYS
1	A	133	PRO
2	B	166	LYS
1	A	2	ILE
2	B	95	PRO
2	B	167	ILE
1	A	18	GLY
2	B	169	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	478/499 (96%)	416 (87%)	62 (13%)	4	19
2	B	368/400 (92%)	321 (87%)	47 (13%)	4	19
All	All	846/899 (94%)	737 (87%)	109 (13%)	4	19

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	5	ILE
1	A	6	GLU
1	A	8	VAL
1	A	21	VAL
1	A	24	TRP
1	A	25	PRO
1	A	26	LEU
1	A	42	GLU
1	A	63	ILE
1	A	65	LYS
1	A	88	TRP
1	A	92	LEU
1	A	113	ASP
1	A	122	GLU
1	A	138	GLU
1	A	142	ILE
1	A	148	VAL
1	A	162	SER
1	A	168	LEU
1	A	184	MET
1	A	185	ASP
1	A	194	GLU
1	A	195	ILE
1	A	197	GLN
1	A	200	THR
1	A	205	LEU
1	A	215	THR
1	A	218	ASP
1	A	228	LEU
1	A	240	THR
1	A	263	LYS
1	A	278	GLN
1	A	283	LEU
1	A	295	LEU
1	A	296	THR
1	A	301	LEU
1	A	303	LEU
1	A	309	ILE
1	A	311	LYS
1	A	340	GLN
1	A	361	HIS

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Mol	Chain	Res	Type
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	423	VAL
1	A	424	LYS
1	A	431	LYS
1	A	448	ARG
1	A	451	LYS
1	A	452	LEU
1	A	465	LYS
1	A	475	GLN
1	A	480	GLN
1	A	488	ASP
1	A	493	VAL
1	A	496	VAL
1	A	514	GLU
1	A	517	LEU
1	A	523	GLU
1	A	527	LYS
1	A	540	LYS
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	24	TRP
2	B	35	VAL
2	B	53	GLU
2	B	63	ILE
2	B	65	LYS
2	B	69	THR
2	B	70	LYS
2	B	84	THR
2	B	87	PHE
2	B	100	LEU
2	B	109	LEU
2	B	122	GLU
2	B	123	ASP
2	B	132	ILE
2	B	161	GLN
2	B	172	ARG
2	B	179	VAL
2	B	184	MET
2	B	186	ASP

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Mol	Chain	Res	Type
2	B	197	GLN
2	B	206	ARG
2	B	214	LEU
2	B	216	THR
2	B	233	GLU
2	B	242	GLN
2	B	245	VAL
2	B	263	LYS
2	B	276	VAL
2	B	280	CYS
2	B	283	LEU
2	B	287	LYS
2	B	289	LEU
2	B	318	TYR
2	B	357	MET
2	B	358	ARG
2	B	361	HIS
2	B	362	THR
2	B	363	ASN
2	B	366	LYS
2	B	368	LEU
2	B	399	GLU
2	B	418	ASN
2	B	425	LEU
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	137	ASN
1	A	174	GLN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	242	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	428	GLN
1	A	475	GLN
1	A	480	GLN
1	A	519	ASN
2	B	57	ASN
2	B	85	GLN
2	B	137	ASN
2	B	147	ASN
2	B	161	GLN
2	B	207	GLN
2	B	242	GLN
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	361	HIS

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	4.59	2 (50%)	1,8,10	4.93	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	8.85	1.55	1.47
1	A	280	CSD	O-C	2.02	1.27	1.20

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.93	114.69	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SBN	A	999	-	21,21,21	3.01	11 (52%)	28,31,31	1.39	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SBN	A	999	-	-	0/14/14/14	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	SBN	C3-C4	8.64	1.47	1.40
3	A	999	SBN	C5-C4	4.39	1.44	1.39
3	A	999	SBN	C10-C11	3.35	1.44	1.39
3	A	999	SBN	C8-C7	3.29	1.44	1.39
3	A	999	SBN	C2-C3	3.20	1.44	1.41
3	A	999	SBN	C7-S	-3.16	1.72	1.77
3	A	999	SBN	C12-C11	3.03	1.43	1.39
3	A	999	SBN	C10-C9	2.88	1.43	1.39
3	A	999	SBN	C4-S	-2.87	1.74	1.78
3	A	999	SBN	C6-C5	2.39	1.43	1.38
3	A	999	SBN	C8-C9	2.30	1.42	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	SBN	C4-C3-C13	-3.24	120.19	123.15
3	A	999	SBN	C5-C4-S	2.57	119.81	116.38
3	A	999	SBN	O2-S-O1	-2.37	114.46	119.25
3	A	999	SBN	C11-C12-C7	2.16	121.64	119.88
3	A	999	SBN	C6-C5-C4	2.03	122.39	118.76

There are no chirality outliers.

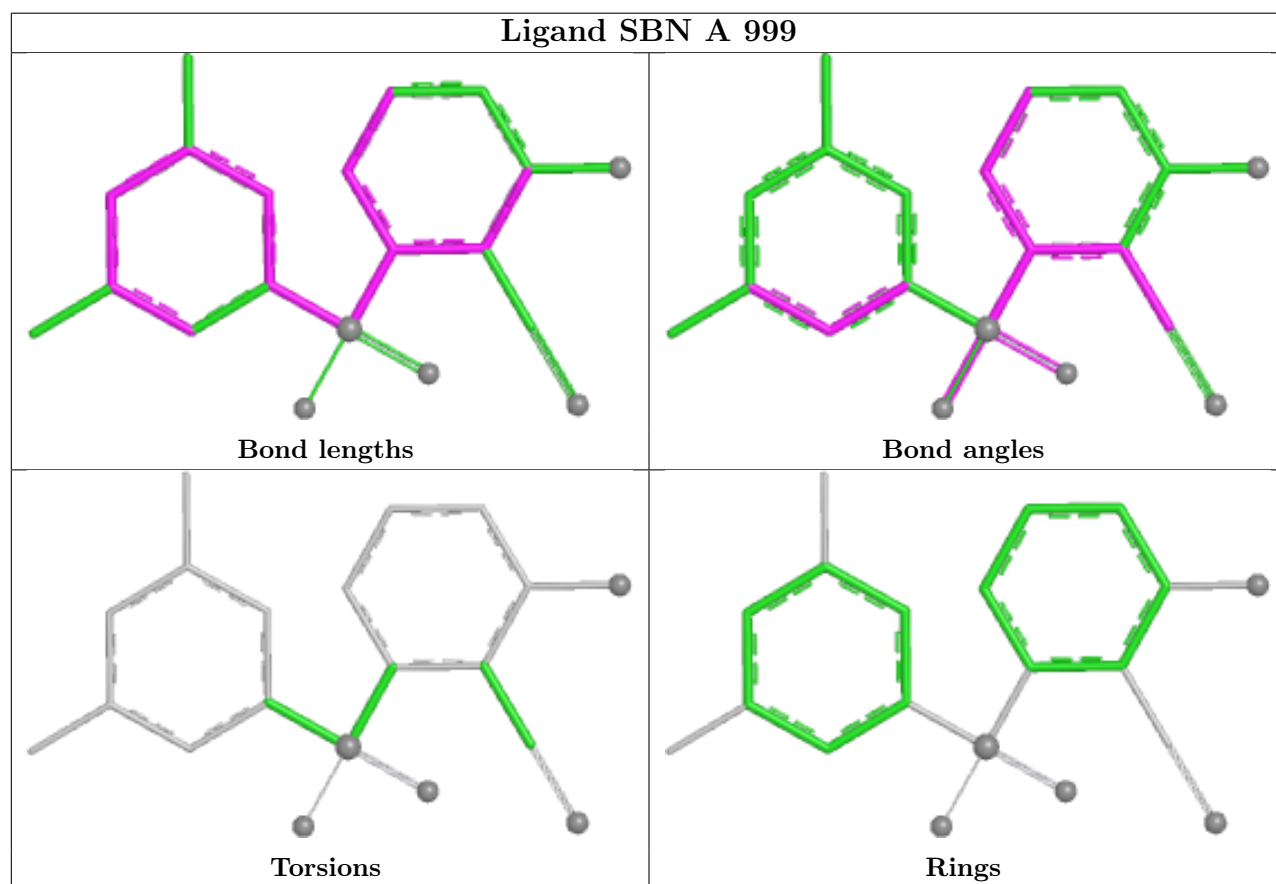
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	SBN	3	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	533/560 (95%)	-0.44	1 (0%) 91 83	34, 86, 136, 150	0
2	B	405/440 (92%)	-0.50	1 (0%) 91 83	41, 82, 134, 150	0
All	All	938/1000 (93%)	-0.46	2 (0%) 91 83	34, 85, 136, 150	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216	THR	2.7
1	A	141	GLY	2.1

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	0.93	0.07	73,78,82,83	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

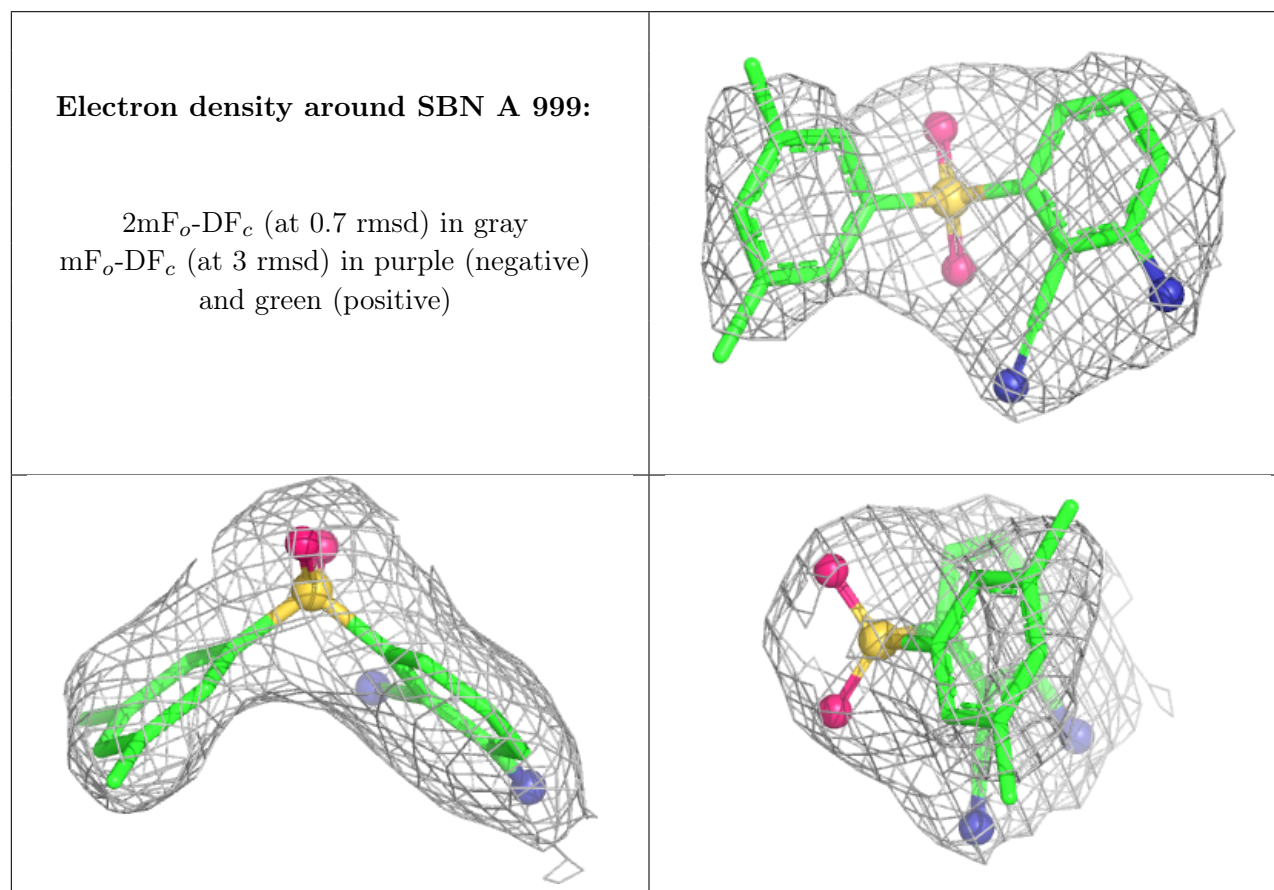
6.4 Ligands [i](#)

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	SBN	A	999	20/20	0.98	0.07	40,56,74,76	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.