



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2022 – 01:34 AM EST

PDB ID : 1JLQ
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH 739W94
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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

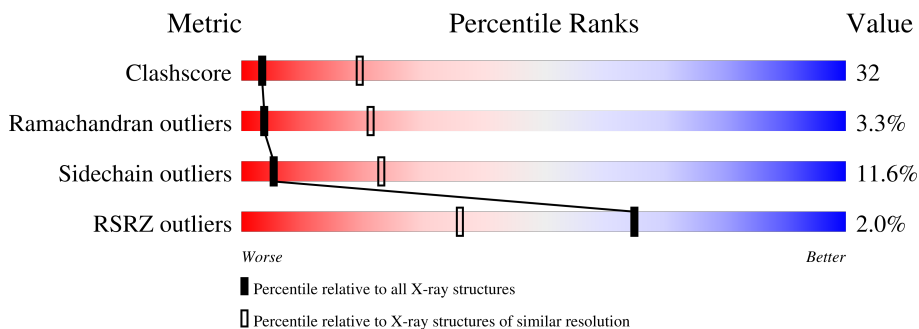
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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	

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
			Total	C	N	O	S			
1	A	534	4363	2823	724	808	8	0	0	0

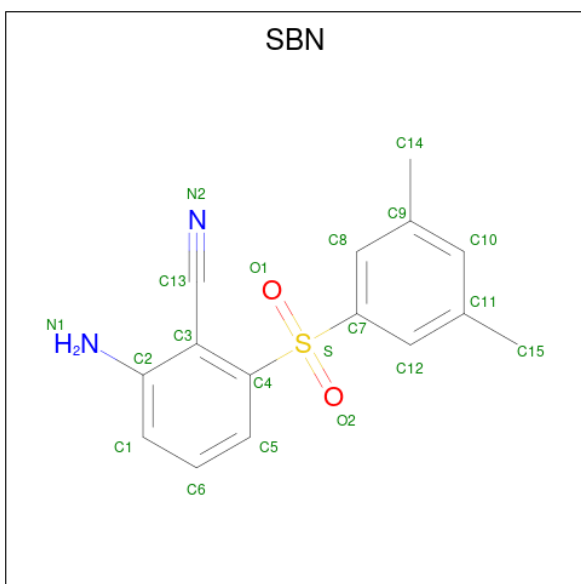
There is a discrepancy between the modelled and reference sequences:

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
			Total	C	N	O	S			
2	B	405	3339	2170	556	606	7	0	0	0

- Molecule 3 is 2-AMINO-6-(3,5-DIMETHYLPHENYL)SULFONYLBENZONITRILE (three-letter code: SBN) (formula: C₁₅H₁₄N₂O₂S).

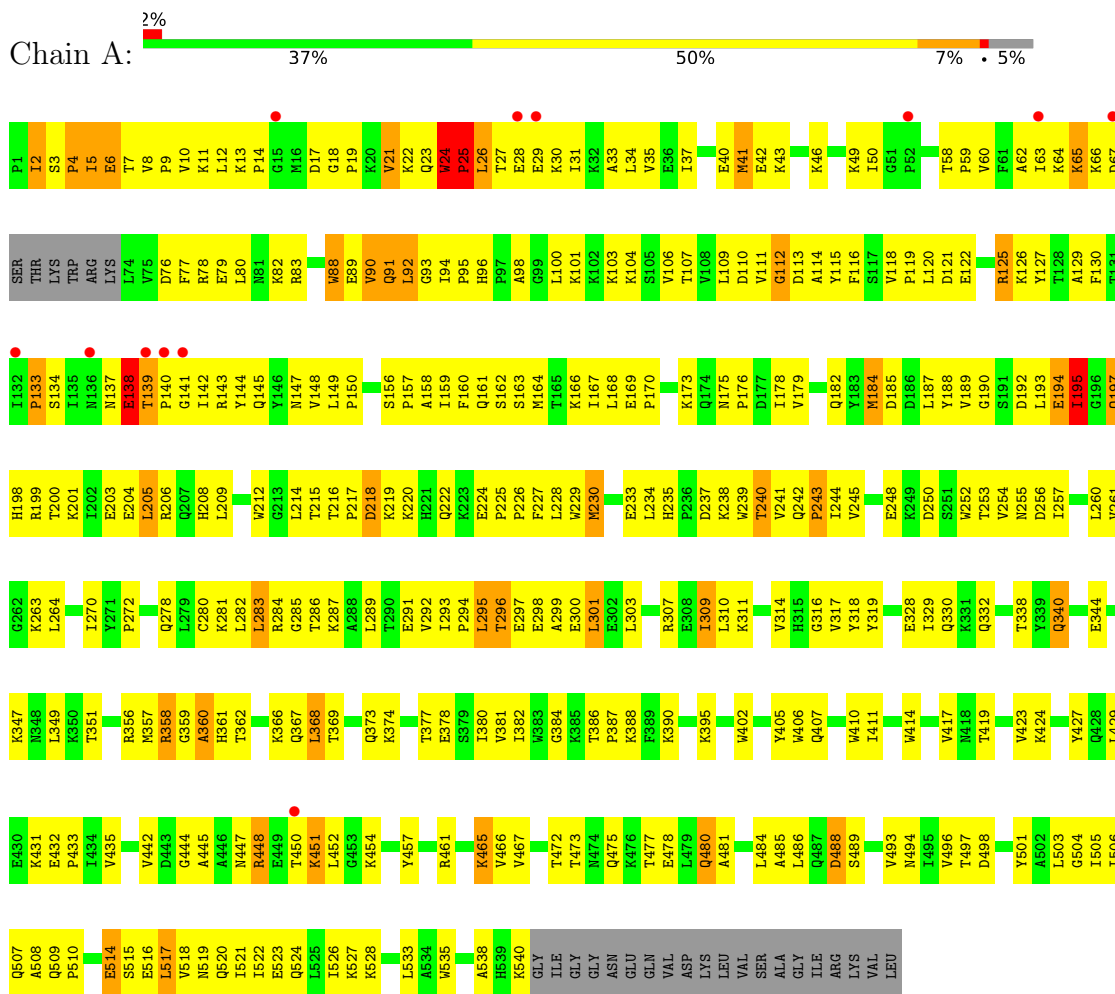


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	20	15	2	2	1	0	0

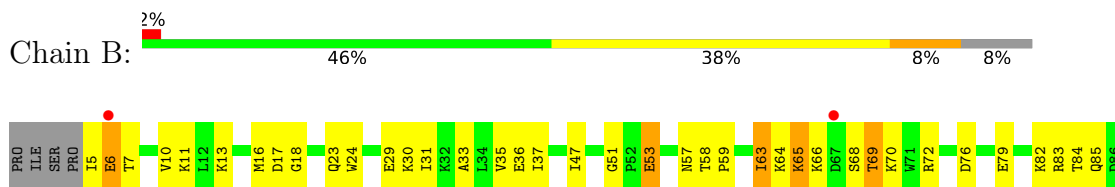
3 Residue-property plots

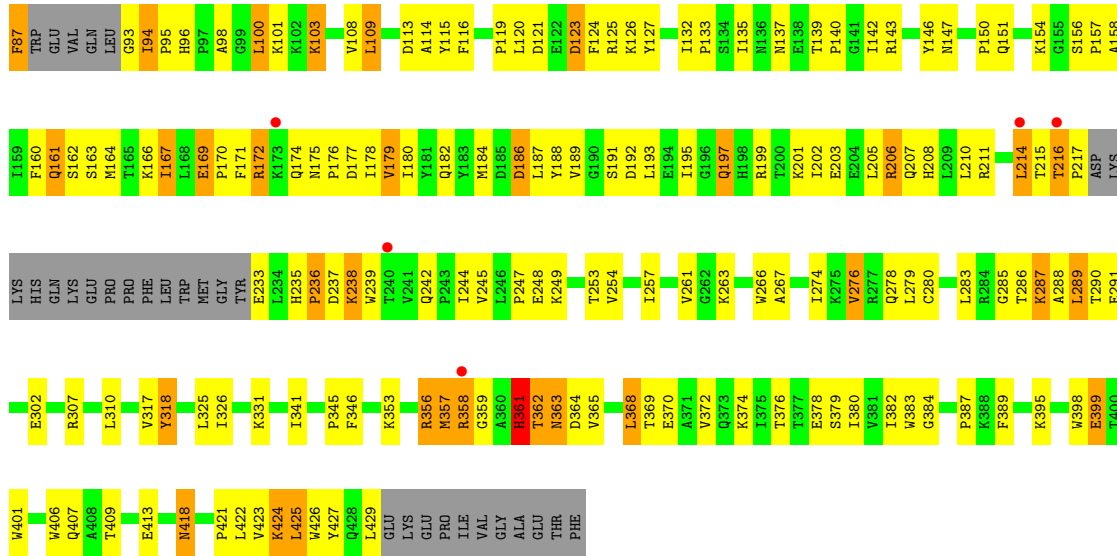
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: HIV-1 RT, A-CHAIN



- Molecule 2: HIV-1 RT, B-CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.10Å 110.90Å 73.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.00 29.88 – 2.98	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.88-3.00) 95.2 (29.88-2.98)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.00Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.267 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SBN, 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	0.49	0/4469	0.73	2/6074 (0.0%)
2	B	0.46	0/3431	0.71	1/4660 (0.0%)
All	All	0.48	0/7900	0.72	3/10734 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	LYS	N-CA-C	-5.66	95.71	111.00
2	B	238	LYS	N-CA-C	-5.36	96.53	111.00
1	A	141	GLY	N-CA-C	-5.21	100.08	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	318	0
2	B	3339	0	3379	195	0
3	A	20	0	14	3	0
All	All	7722	0	7798	502	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 32.

All (502) 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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:GLU:H	1:A:122:GLU:CD	1.94	0.70
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
2:B:79:GLU:O	2:B:83:ARG:HG3	1.94	0.68
1:A:199:ARG:HD3	1:A:219:LYS:HZ1	1.59	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:507:GLN:C	1:A:509:GLN:H	2.00	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: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:33:ALA:O	1:A:37:ILE:HD13	1.99	0.61
1:A:300:GLU:OE2	1:A:300:GLU:HA	2.00	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: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:199:ARG:HG3	1:A:219:LYS:HZ3	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:LYS:C	2:B:68:SER:H	2.04	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:37:ILE:O	1:A:40:GLU:HB3	2.02	0.59
1:A:24:TRP:O	1:A:25:PRO:C	2.40	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
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: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
1:A:27:THR:CG2	1:A:28:GLU:N	2.68	0.57
1:A:507:GLN:C	1:A:509:GLN:N	2.58	0.57
1:A:270:ILE:O	1:A:272:PRO:HD3	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:N	2:B:176:PRO:HD3	2.20	0.56
1:A:292:VAL:C	1:A:293:ILE:HD12	2.25	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:184:MET:HA	1:A:184:MET:CE	2.37	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: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
2:B:206:ARG:C	2:B:210:LEU:HD13	2.26	0.55
1:A:122:GLU:HA	1:A:125:ARG:NE	2.22	0.55
1:A:199:ARG:CD	1:A:219:LYS:HZ1	2.20	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
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
1:A:472:THR:OG1	1:A:473:THR:N	2.40	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:229:TRP:O	1:A:230:MET:C	2.47	0.53
1:A:158:ALA:O	1:A:161:GLN:HB3	2.09	0.53
1:A:7:THR:HG22	1:A:119:PRO:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:236:PRO:C	2:B:238:LYS:H	2.13	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
1:A:503:LEU:O	1:A:504:GLY:C	2.46	0.52
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:318:TYR:O	1:A:349:LEU:HD21	2.12	0.50
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: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
2:B:66:LYS:C	2:B:68:SER:N	2.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ASP:O	2:B:114:ALA:C	2.51	0.48
1:A:239:TRP:HZ3	1:A:241:VAL:HG23	1.78	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
1:A:332:GLN:HG2	1:A:338:THR:HG23	1.95	0.48
1:A:134:SER:HB3	1:A:138:GLU:HG2	1.95	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
1:A:160:PHE:CZ	1:A:164:MET:HE3	2.49	0.48
2:B:193:LEU:H	2:B:193:LEU:CD1	2.27	0.48
1:A:110:ASP:C	1:A:112:GLY:H	2.16	0.48
1:A:195:ILE:O	1:A:198:HIS:HB3	2.13	0.48
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: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: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
2:B:383:TRP:O	2:B:384:GLY:C	2.53	0.47
2:B:427:TYR:C	2:B:429:LEU:N	2.68	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
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: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: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
1:A:88:TRP:CG	1:A:89:GLU:N	2.83	0.46
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:O	1:A:167:ILE:HG13	2.15	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:498:ASP:C	1:A:535:TRP:HE1	2.18	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.45	0.46
2:B:207:GLN:HA	2:B:210:LEU:HD22	1.98	0.46
2:B:422:LEU:C	2:B:424:LYS:N	2.69	0.46
1:A:254:VAL:O	1:A:255:ASN:C	2.53	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
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:493:VAL:HG12	1:A:494:ASN:H	1.81	0.45
1:A:285:GLY:O	1:A:286:THR:C	2.55	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
1:A:317:VAL:CG1	1:A:318:TYR:N	2.79	0.45
2:B:98:ALA:HA	2:B:101:LYS:HD2	1.99	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:373:GLN:HG3	1:A:374:LYS:N	2.32	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:184:MET:HA	1:A:184:MET:HE2	1.99	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:65:LYS:H	1:A:65:LYS:CD	2.25	0.44
1:A:218:ASP:C	1:A:220:LYS:N	2.70	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
2:B:236:PRO:C	2:B:238:LYS:N	2.71	0.44
1:A:5:ILE:HD11	1:A:166:LYS:NZ	2.31	0.44
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.00	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
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
2:B:424:LYS:HD2	2:B:424:LYS:C	2.38	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
2:B:363:ASN:OD1	2:B:363:ASN:C	2.56	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: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
1:A:194:GLU:O	1:A:195:ILE:C	2.56	0.43
1:A:203:GLU:O	1:A:204:GLU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:35:VAL:HG23	2:B:132:ILE:HG21	2.01	0.43
2:B:427:TYR:C	2:B:429:LEU:H	2.22	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:64:LYS:CE	1:A:66:LYS:HZ1	2.32	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:270:ILE:C	1:A:272:PRO:HD3	2.40	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:367:GLN:O	1:A:368:LEU:C	2.58	0.42
1:A:405:TYR:O	2:B:331:LYS:HD3	2.19	0.42
1:A:497:THR:O	1:A:535:TRP:HA	2.18	0.42
2:B:53:GLU:CD	2:B:53:GLU:H	2.22	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:64:LYS:CE	1:A:66:LYS:NZ	2.82	0.42
1:A:106:VAL:HG12	1:A:107:THR:N	2.34	0.42
1:A:110:ASP:C	1:A:112:GLY:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:C	2:B:177:ASP:H	2.23	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
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
2:B:205:LEU:HD13	2:B:205:LEU:C	2.40	0.42
1:A:77:PHE:O	1:A:78:ARG:C	2.58	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
2:B:65:LYS:HE2	2:B:72:ARG:HD3	2.02	0.41
2:B:422:LEU:C	2:B:424:LYS:H	2.23	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
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: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
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
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:359:GLY:O	1:A:360:ALA:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/560 (94%)	452 (85%)	58 (11%)	19 (4%)	3	19
2	B	399/440 (91%)	342 (86%)	45 (11%)	12 (3%)	4	24
All	All	928/1000 (93%)	794 (86%)	103 (11%)	31 (3%)	4	21

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	91	GLN
1	A	138	GLU
1	A	195	ILE
2	B	215	THR

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Mol	Chain	Res	Type
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 [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	478/499 (96%)	420 (88%)	58 (12%)	5	21
2	B	368/400 (92%)	328 (89%)	40 (11%)	6	25
All	All	846/899 (94%)	748 (88%)	98 (12%)	5	23

All (98) 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	11	LYS
1	A	21	VAL
1	A	24	TRP
1	A	25	PRO
1	A	26	LEU
1	A	41	MET
1	A	63	ILE
1	A	65	LYS
1	A	92	LEU
1	A	113	ASP
1	A	138	GLU
1	A	162	SER
1	A	182	GLN
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	250	ASP
1	A	263	LYS
1	A	283	LEU
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	301	LEU
1	A	303	LEU
1	A	309	ILE
1	A	311	LYS
1	A	340	GLN
1	A	357	MET
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	423	VAL

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Mol	Chain	Res	Type
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	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	10	VAL
2	B	24	TRP
2	B	53	GLU
2	B	63	ILE
2	B	65	LYS
2	B	69	THR
2	B	70	LYS
2	B	87	PHE
2	B	100	LEU
2	B	109	LEU
2	B	123	ASP
2	B	161	GLN
2	B	172	ARG
2	B	179	VAL
2	B	186	ASP
2	B	197	GLN
2	B	206	ARG
2	B	211	ARG
2	B	214	LEU
2	B	216	THR
2	B	233	GLU
2	B	242	GLN
2	B	263	LYS
2	B	276	VAL
2	B	280	CYS
2	B	283	LEU

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Mol	Chain	Res	Type
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	368	LEU
2	B	399	GLU
2	B	418	ASN
2	B	424	LYS
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	96	HIS
1	A	137	ASN
1	A	174	GLN
1	A	197	GLN
1	A	222	GLN
1	A	242	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	367	GLN
1	A	475	GLN
1	A	480	GLN
1	A	519	ASN
2	B	57	ASN
2	B	85	GLN
2	B	161	GLN
2	B	207	GLN
2	B	242	GLN
2	B	278	GLN
2	B	330	GLN
2	B	340	GLN
2	B	361	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	3,7,8	1.34	0	1,8,10	4.81	1 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.81	114.69	105.54

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 monosaccharides 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	-	19,21,21	2.25	8 (42%)	27,31,31	1.28	2 (7%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	SBN	C5-C4	4.35	1.44	1.39
3	A	999	SBN	C8-C7	3.21	1.44	1.39
3	A	999	SBN	C10-C11	3.13	1.44	1.39
3	A	999	SBN	C7-S	-3.12	1.72	1.77
3	A	999	SBN	C4-S	-2.85	1.74	1.78
3	A	999	SBN	C12-C11	2.84	1.43	1.39
3	A	999	SBN	C10-C9	2.70	1.43	1.39
3	A	999	SBN	C8-C9	2.16	1.42	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	SBN	O2-S-O1	-2.50	114.46	119.23
3	A	999	SBN	C5-C4-S	2.27	119.81	116.40

There are no chirality outliers.

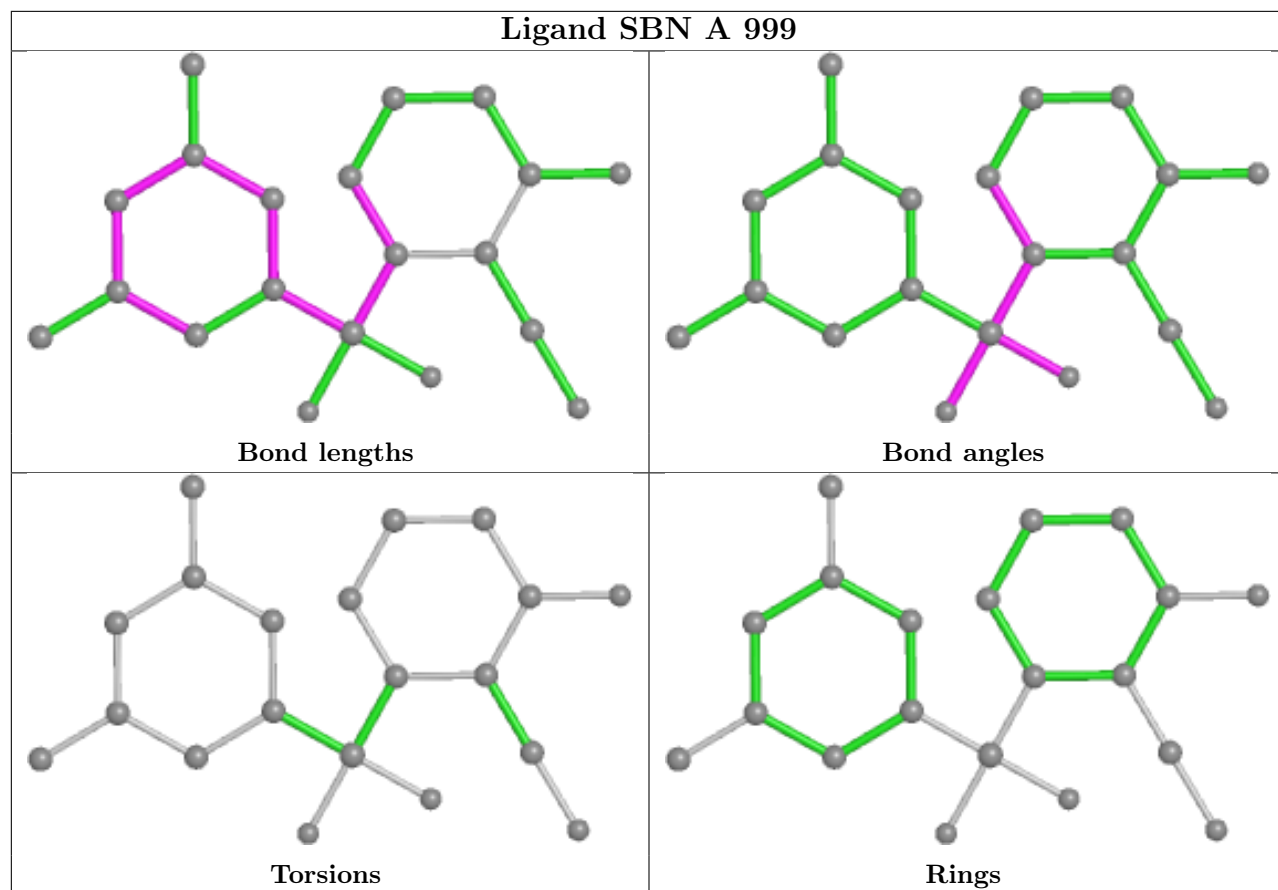
There are no torsion outliers.

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	533/560 (95%)	-0.35	12 (2%) 60 31	34, 86, 136, 150	0
2	B	405/440 (92%)	-0.38	7 (1%) 70 41	41, 82, 134, 150	0
All	All	938/1000 (93%)	-0.36	19 (2%) 65 36	34, 85, 136, 150	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	GLY	5.8
1	A	139	THR	4.5
1	A	28	GLU	3.8
1	A	67	ASP	3.6
1	A	140	PRO	3.3
2	B	216	THR	3.2
2	B	6	GLU	2.9
1	A	450	THR	2.7
2	B	67	ASP	2.7
1	A	15	GLY	2.7
1	A	29	GLU	2.5
2	B	173	LYS	2.4
1	A	52	PRO	2.3
1	A	132	ILE	2.2
2	B	214	LEU	2.1
1	A	136	ASN	2.1
2	B	240	THR	2.1
1	A	63	ILE	2.1
2	B	358	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.91	0.17	73,78,82,83	0

6.3 Carbohydrates [i](#)

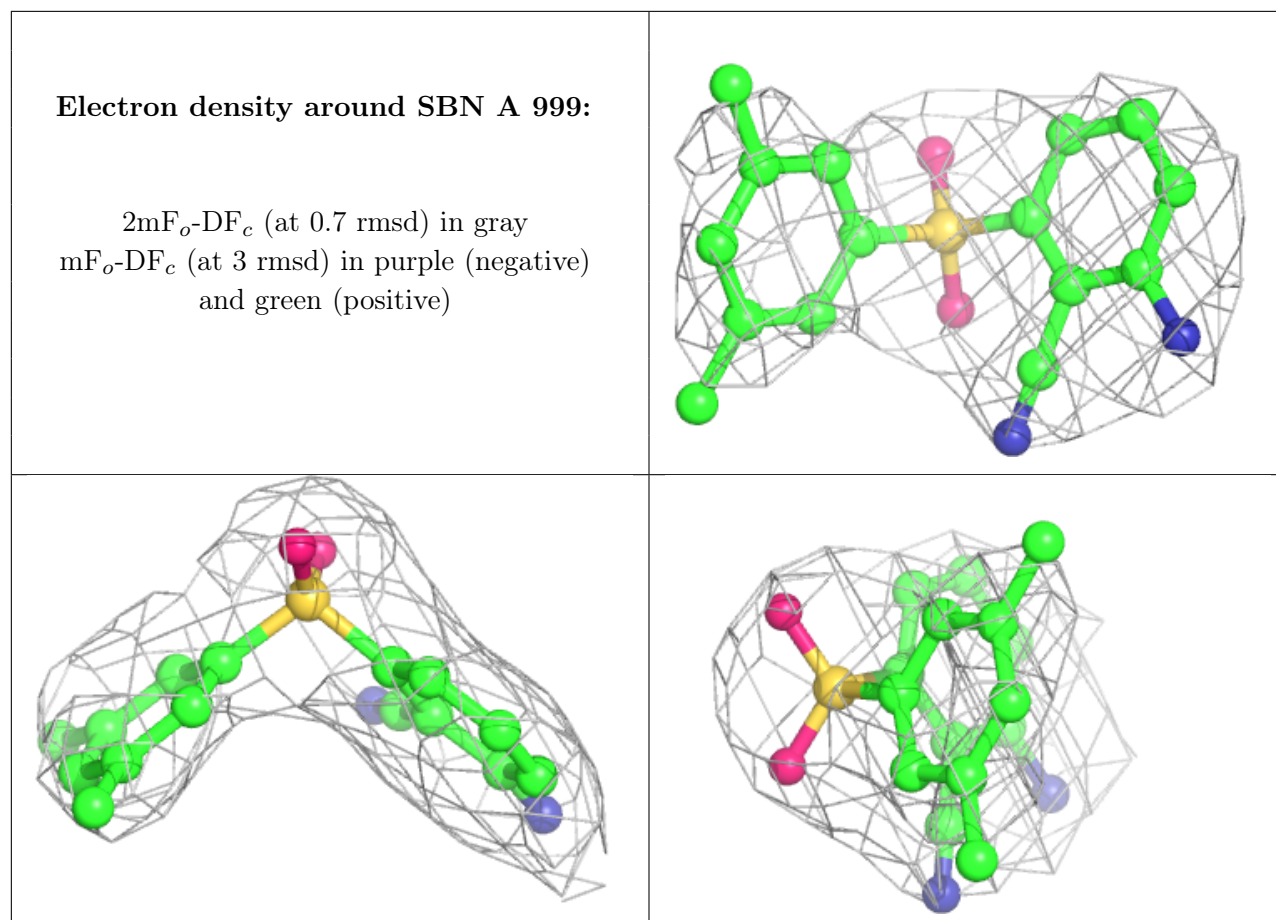
There are no monosaccharides in this entry.

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	0.18	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.